

## Supplementary information for “Designing strategies to tune reduction potential of organic molecules for sustainable high capacity batteries application.”

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**Content: Molecular geometries investigated in this work. The molecules' numbers are the same as in the main paper.**

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#####mol1#####  
#####mol#####  
12  
structure  
C1      -0.3872058658  -1.7841529204  0.0771053854  
C2      -0.3698923518  -0.3903129237  0.0740973456  
C3       0.8457415834  0.2916517303  0.0902056759  
C4       2.0440599502  -0.4202264730  0.1093218292  
C5       2.0267472408  -1.8140652246  0.1123310101  
C6       0.8111140485  -2.4960300447  0.0962227769  
H7      -1.3329166857  -2.3146840677  0.0645749377  
H8      -1.3021329893  0.1634886000  0.0592263004  
H9       0.8592130055  1.3759945793  0.0878657036  
H10     2.9897720109  0.1103035070  0.1218508235  
H11     2.9589880073  -2.3678670658  0.1272025031  
H12     0.7976463506  -3.5803732657  0.0985634560  
#####mol_reduced#####  
12
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structure

C1	-0.3868743506	-1.7965261150	0.0771386034
C2	-0.4119307205	-0.3773806834	0.0734566008
C3	0.8672741578	0.3118480895	0.0904720095
C4	2.0437285037	-0.4078514052	0.1092894126
C5	2.0687808354	-1.8269984550	0.1129705519
C6	0.7895851417	-2.5162249434	0.0959569301
H7	-1.3345613130	-2.3398244026	0.0646100627
H8	-1.3492083390	0.1703059464	0.0585253987
H9	0.8987238528	1.4007535387	0.0883816050
H10	2.9914454746	0.1353914968	0.1218179785
H11	3.0060649246	-2.3746669586	0.1278991894
H12	0.7581174560	-3.6051252374	0.0980484767

#####mol\_double\_reduced#####

12

structure

C1	-0.3913004138	-1.7872937377	0.0724520660
C2	-0.4073142221	-0.3930648547	0.1612850284
C3	0.8699517586	0.3183839200	0.0068035457
C4	2.0482720781	-0.4170415605	0.1065862295
C5	2.0614947665	-1.8108415580	0.2016567788
C6	0.7893952965	-2.5231944664	0.0123290490
H7	-1.3844428252	-2.3485731813	0.0392818123
H8	-1.3111811540	0.1032777956	0.6041921989
H9	0.9251397283	1.3466086519	-0.4432894261
H10	3.0419947682	0.1441280830	0.0989369744
H11	2.9516984316	-2.3059269405	0.6723789715
H12	0.7481387601	-3.5536475179	-0.4339905168

#####mol2#####

#####mol#####

18

structure

C1	-1.5929208313	0.8353959643	0.1170179469
C2	-1.5910685360	-0.5790765579	0.1346881519
C3	-0.4042653649	-1.2702145359	0.1283784520
C4	0.8378274952	-0.5845830820	0.1041485586
C5	0.8359527027	0.8465121355	0.0862835190
C6	-0.4079353263	1.5292703092	0.0934174662
C7	2.0780373394	1.5321512976	0.0620619174
C8	3.2648465888	0.8410192460	0.0557570205
C9	3.2667014910	-0.5734500617	0.0734218290
C10	2.0817144574	-1.2673365324	0.0970138794
H11	-2.5358801724	1.3703066886	0.1222060761
H12	-2.5326250810	-1.1161529742	0.1532802038
H13	-0.4015695743	-2.3553029892	0.1419237464
H14	-0.4080887328	2.6143624754	0.0798566064
H15	2.0753487896	2.6172378519	0.0485230042
H16	4.2064072956	1.3780940245	0.0371737734
H17	4.2096702714	-1.1083479086	0.0682392010

H18 2.0818877355 -2.3524255302 0.1105792868  
#####mol\_reduced#####

18

structure

C1	-1.6316944805	0.8221082099	0.1176692009
C2	-1.6298685160	-0.5658854563	0.1350101454
C3	-0.4107884507	-1.2704476838	0.1284686319
C4	0.8378486214	-0.5947132447	0.1042808699
C5	0.8359396582	0.8566533817	0.0861565817
C6	-0.4144730019	1.5294924301	0.0934973561
C7	2.0845646863	1.5323943135	0.0619762549
C8	3.3036463179	0.8278169819	0.0554324693
C9	3.3054697407	-0.5601674219	0.0727640050
C10	2.0882424293	-1.2675619810	0.0969352012
H11	-2.5731230453	1.3674889936	0.1227081729
H12	-2.5698596971	-1.1134416989	0.1537076998
H13	-0.4111433567	-2.3582137630	0.1420866175
H14	-0.4176923161	2.6172544104	0.0799360345
H15	2.0849685867	2.6201582030	0.0483675893
H16	4.2436358007	1.3753806701	0.0367401795
H17	4.2468995801	-1.1055484167	0.0677211241
H18	2.0915008317	-2.3553227938	0.1104909602

#####mol\_double\_reduced#####

18

structure

C1	-1.6775186606	0.8136304243	0.1183550145
C2	-1.6757117800	-0.5575184070	0.1354811231
C3	-0.4221453316	-1.2712336590	0.1286166821
C4	0.8378587772	-0.6054909218	0.1044166135
C5	0.8359026432	0.8674121569	0.0860206208
C6	-0.4258223827	1.5302325711	0.0936216527
C7	2.0958970329	1.5331732297	0.0618374718
C8	3.3494986174	0.8194683078	0.0549622789
C9	3.3513233319	-0.5516817664	0.0720741859
C10	2.0996097854	-1.2683063734	0.0968046999
H11	-2.6193441489	1.3722360119	0.1232482208
H12	-2.6160717266	-1.1182928341	0.1543448429
H13	-0.4290938302	-2.3650126684	0.1423978905
H14	-0.4356387777	2.6239957558	0.0800504069
H15	2.1028308281	2.6269599658	0.0480785083
H16	4.2898430839	1.3802779010	0.0360991357
H17	4.2931492176	-1.1102929213	0.0671701025
H18	2.1094518653	-2.3620683703	0.1103737135

#####mol3#####

#####mol#####

24

structure

C1	-2.8256692718	-0.3770357600	0.0791992941
C2	-2.8353144867	-1.8013185382	0.0812865974

C3	-1.6619494357	-2.5014299573	0.0902014278
C4	-0.4029637918	-1.8270738088	0.0976213064
C5	-0.3931917632	-0.3841631654	0.0955094728
C6	-1.6429282261	0.3071479202	0.0860890458
C7	0.8328704442	0.2872860993	0.1027108494
C8	2.0497612466	-0.4006707175	0.1118995454
C9	2.0399934584	-1.8435693562	0.1140026710
C10	0.8139059668	-2.5150254309	0.1068045612
C11	3.2897154799	-2.5348856392	0.1234156743
C12	4.4724619695	-1.8506943221	0.1303100162
C13	4.4821014238	-0.4264176922	0.1282335608
C14	3.3087292098	0.2736942093	0.1193225205
H15	-3.7660893483	0.1623729619	0.0720784649
H16	-3.7829520896	-2.3279657715	0.0757280115
H17	-1.6690657641	-3.5864677043	0.0917906283
H18	-1.6353456293	1.3921802728	0.0844977587
H19	0.8402429669	1.3731915432	0.1011279119
H20	0.8065958229	-3.6009309407	0.1083843589
H21	3.2821475942	-3.6199164211	0.1249968798
H22	5.4128997980	-2.3900771075	0.1374261976
H23	5.4297419286	0.1002281840	0.1337984032
H24	3.3158683117	1.3587296898	0.1177409198

#####mol\_reduced#####

24

structure

C1	-2.8670048010	-0.3882401135	0.0789447866
C2	-2.8764962068	-1.7895590049	0.0809876986
C3	-1.6747474845	-2.4924899736	0.0900931466
C4	-0.4204589735	-1.8305453233	0.0975028241
C5	-0.4106587562	-0.3804990190	0.0953913243
C6	-1.6558471848	0.2983556641	0.0860306647
C7	0.8328491943	0.2868443945	0.1027127390
C8	2.0672637240	-0.3972005986	0.1120061482
C9	2.0574621738	-1.8472364716	0.1141271312
C10	0.8139236330	-2.5145845904	0.1067984273
C11	3.3026240329	-2.5260929220	0.1235014678
C12	4.5137963560	-1.8394827147	0.1305800334
C13	4.5232868585	-0.4381809950	0.1285212188
C14	3.3215204984	0.2647579818	0.1194083855
H15	-3.8035278111	0.1632155227	0.0718318213
H16	-3.8204158791	-2.3282708324	0.0754680724
H17	-1.6826591349	-3.5800761454	0.0916711379
H18	-1.6490014810	1.3859467875	0.0844431892
H19	0.8402564900	1.3749532294	0.1011281174
H20	0.8066370357	-3.6026942838	0.1083815053
H21	3.2958574759	-3.6136830509	0.1251009957
H22	5.4503053916	-2.3909628634	0.1377004795
H23	5.4671996779	0.1005451945	0.1340328051
H24	3.3295008879	1.3523417020	0.1178179203

#####mol\_double\_reduced#####

24

structure

C1	-2.9129811034	-0.3960104001	0.0786432837
C2	-2.9223543264	-1.7811708751	0.0806865263
C3	-1.6925121421	-2.4889695492	0.0899876634
C4	-0.4375136100	-1.8355303045	0.0973961092
C5	-0.4276337796	-0.3752229371	0.0952569867
C6	-1.6736774852	0.2951100702	0.0858895060
C7	0.8327962007	0.2791619600	0.1027198279
C8	2.0843429081	-0.3922037204	0.1121189820
C9	2.0744572228	-1.8525143855	0.1142409667
C10	0.8139481595	-2.5068951074	0.1067778140
C11	3.3204294532	-2.5228741706	0.1235987511
C12	4.5597658062	-1.8317091476	0.1308679292
C13	4.5691452282	-0.4465788677	0.1288583368
C14	3.3392722268	0.2612574432	0.1195602980
H15	-3.8489241985	0.1660589225	0.0715187137
H16	-3.8658190127	-2.3305408924	0.0752056111
H17	-1.7025961001	-3.5807533781	0.0915736595
H18	-1.6689953563	1.3869292448	0.0842636055
H19	0.8403392876	1.3721592746	0.1011209799
H20	0.8067086665	-3.5998869287	0.1083671653
H21	3.3159683936	-3.6146895667	0.1252106810
H22	5.4956506935	-2.3938790993	0.1379896293
H23	5.5125845510	0.1028398704	0.1343627547
H24	3.3495727547	1.3530338266	0.1179991466

#####mol4#####

#####mol#####

24

structure

C1	4.3787527954	-0.5443979850	0.0778879715
C2	3.7007953841	-1.7747684276	0.0832833733
C3	2.3210900762	-1.8112289690	0.0937310019
C4	1.5514899765	-0.6266017303	0.0992971935
C5	2.2449162488	0.6174833634	0.0937843760
C6	3.6570400617	0.6290618690	0.0830940995
C7	1.5025170315	1.8434903768	0.0991453115
C8	0.1463940835	1.8441680753	0.1094241605
C9	-0.5972438091	0.6189111564	0.1153274146
C10	0.0949393094	-0.6258739535	0.1103334896
C11	-0.6758178974	-1.8097290444	0.1164145768
C12	-2.0554854895	-1.7718733788	0.1268927788
C13	-2.7322199307	-0.5408250882	0.1318014510
C14	-2.0093467492	0.6319215238	0.1260682367
H15	5.4624461696	-0.5203477950	0.0696785809
H16	4.2627944951	-2.7018742231	0.0792279269
H17	1.8287918075	-2.7749229020	0.0976688784
H18	4.1684732757	1.5861076661	0.0790108874

H19	2.0525467214	2.7787414218	0.0947795759
H20	-0.4027322126	2.7799582909	0.1133906598
H21	-0.1844860087	-2.7739160176	0.1128676571
H22	-2.6184228202	-2.6984088244	0.1313584372
H23	-3.8158898135	-0.5157157056	0.1400471912
H24	-2.5198345143	1.5894709383	0.1297710909

#####mol\_reduced#####

24

structure

C1	4.3989245641	-0.5618288508	0.0777462775
C2	3.7279191598	-1.7930875370	0.0830921367
C3	2.3250147993	-1.7979341213	0.0937024730
C4	1.5624779372	-0.6255611503	0.0992084856
C5	2.2561362890	0.6462991088	0.0936833269
C6	3.6893294033	0.6219036334	0.0828443046
C7	1.5271768607	1.8458379725	0.0989459001
C8	0.1217738203	1.8465082580	0.1096125538
C9	-0.6084173431	0.6477141944	0.1154117678
C10	0.0839542063	-0.6248547876	0.1104036352
C11	-0.6797302377	-1.7964456146	0.1164247573
C12	-2.0826763215	-1.7901530303	0.1271000671
C13	-2.7524223640	-0.5582429041	0.1319725690
C14	-2.0416228219	0.6248017720	0.1263320402
H15	5.4868034843	-0.5372576413	0.0695178084
H16	4.2795354933	-2.7277448180	0.0791314605
H17	1.8204016276	-2.7582515450	0.0977384618
H18	4.2160258719	1.5732028834	0.0786483784
H19	2.0720163628	2.7867039359	0.0946138642
H20	-0.4222206581	2.7878774892	0.1135493378
H21	-0.1761989532	-2.7573276368	0.1127746375
H22	-2.6351810139	-2.7242848123	0.1314798586
H23	-3.8402785043	-0.5325661549	0.1402536644
H24	-2.5674173658	1.5765975594	0.1301546217

#####mol\_double\_reduced#####

24

structure

C1	4.4316672904	-0.5779150838	0.0774411025
C2	3.7403243275	-1.7908627869	0.0829788263
C3	2.3336935107	-1.8177185148	0.0936780577
C4	1.5414814545	-0.6143079536	0.0994074184
C5	2.2734844011	0.6533975124	0.0935678228
C6	3.6988331303	0.6332383177	0.0827325793
C7	1.5298521048	1.8516439061	0.0989561463
C8	0.1190798292	1.8523387223	0.1096650487
C9	-0.6257702707	0.6548501765	0.1155630858
C10	0.1049425004	-0.6136115322	0.1102844437
C11	-0.6884261253	-1.8162290466	0.1165194277
C12	-2.0950462310	-1.7879316267	0.1271728946
C13	-2.7851514493	-0.5742895190	0.1321669397

C14	-2.0511264640	0.6361530746	0.1263661363
H15	5.5231902505	-0.5603324077	0.0691341080
H16	4.2926939308	-2.7337433952	0.0789974903
H17	1.8341825545	-2.7813535539	0.0977130030
H18	4.2244794144	1.5900131716	0.0785178299
H19	2.0728311955	2.7993805014	0.0946375685
H20	-0.4230333631	2.8005847843	0.1135840617
H21	-0.1899313992	-2.7803868699	0.1129116238
H22	-2.6483932807	-2.7302409219	0.1315488540
H23	-3.8766629560	-0.5556187238	0.1404358274
H24	-2.5758706783	1.5934161720	0.1301479355

#####mol5#####

#####mol#####

22

structure

C1	-1.3700403341	3.5981991867	0.5191933978
C2	-1.3701818507	2.2067255341	0.5250543390
C3	-0.2469228563	1.4833248550	0.0987292368
C4	0.8768574641	2.2022731116	-0.3337091439
C5	0.8777045005	3.5937491026	-0.3396732986
C6	-0.2459192848	4.2982451070	0.0867722802
C7	-0.2474509796	-0.0021009452	0.1050118975
C8	0.8872017801	-0.7219801577	0.5063865372
C9	0.8870854739	-2.1134557226	0.5122899073
C10	-0.2484153747	-2.8170143288	0.1168920575
C11	-1.3834392226	-2.1160391578	-0.2844237284
C12	-1.3826055370	-0.7245645124	-0.2902627347
H13	-2.2469038887	4.1365846456	0.8614349108
H14	-2.2413238659	1.6728639781	0.8873486707
H15	1.7476158214	1.6647318003	-0.6914641240
H16	1.7549499130	4.1285826153	-0.6864789950
H17	-0.2455346765	5.3822871253	0.0821613562
H18	1.7679016035	-0.1851614447	0.8400810034
H19	1.7731002787	-2.6490163628	0.8348307471
H20	-0.2487816831	-3.9010565329	0.1214570715
H21	-2.2698173146	-2.6536925910	-0.6024456853
H22	-2.2629368080	-0.1899760875	-0.6284757525

#####mol\_reduced#####

22

structure

C1	-1.4426092658	3.6205884113	0.2038507890
C2	-1.4501973489	2.2395481830	0.2080355573
C3	-0.2463557177	1.4591829755	0.0988943003
C4	0.9573887274	2.2387539015	-0.0174274073
C5	0.9498863727	3.6197246151	-0.0240119219
C6	-0.2464344877	4.3547732233	0.0870376638
C7	-0.2468626655	0.0220367293	0.1045765030
C8	0.9590019540	-0.7585059833	0.1878028712
C9	0.9505413279	-2.1394722004	0.1949744847

C10	-0.2489861212	-2.8735311670	0.1170137286
C11	-1.4473294083	-2.1383753487	0.0328884091
C12	-1.4538843748	-0.7573465807	0.0285396574
H13	-2.3892324013	4.1493483607	0.3032583350
H14	-2.4015233906	1.7340765319	0.3315910726
H15	1.9087832658	1.7323868632	-0.1363174940
H16	1.8963739198	4.1477244261	-0.1285409862
H17	-0.2464442660	5.4395701247	0.0821433617
H18	1.9137069893	-0.2529066209	0.2805618968
H19	1.8991049339	-2.6682381822	0.2736142152
H20	-0.2499031268	-3.9583254988	0.1222812121
H21	-2.3967149216	-2.6664403909	-0.0404063782
H22	-2.4078063488	-0.2510318343	-0.0688094138

#####mol\_double\_reduced#####

22

structure

C1	-1.4497556675	3.6302233756	0.1060268614
C2	-1.4698675293	2.2596560720	-0.0010503935
C3	-0.2476239904	1.4357514479	0.0506558955
C4	0.9735080870	2.2585218916	-0.0337512190
C5	0.9574896962	3.6291259097	0.0735070842
C6	-0.2437896684	4.3800021170	0.2383469648
C7	-0.2467341205	0.0453784953	0.1524595672
C8	0.9754788641	-0.7783294874	0.2047006088
C9	0.9554602662	-2.1489602249	0.0975788074
C10	-0.2504640441	-2.8986873154	-0.0347877003
C11	-1.4518694352	-2.1479292533	0.1303145971
C12	-1.4678663861	-0.7774085064	0.2381325698
H13	-2.4050060005	4.1664904901	0.0541594563
H14	-2.4245681928	1.7671509724	-0.1804179982
H15	1.9225140114	1.7653708882	-0.2398202144
H16	1.9113276989	4.1647040495	-0.0044258681
H17	-0.2425888682	5.4678549888	0.2682007525
H18	1.9300833427	-0.2859091135	0.3849488281
H19	1.9106168815	-2.6852525251	0.1504745267
H20	-0.2515481538	-3.9865106610	-0.0650916806
H21	-2.4055524440	-2.6837859780	0.2085632367
H22	-2.4166365552	-0.2835654896	0.4432728670

#####mol6#####

#####mol#####

11

structure

C1	0.2485267201	0.1679994477	0.0871964928
C2	-1.2550885770	0.1142171164	0.0706507304
C3	-1.7407666134	1.3695149322	0.0809420356
C4	-0.6233826912	2.3222205201	0.1041055868
C5	0.5393610834	1.6442054871	0.1079314434
H6	0.6867189799	-0.3245139704	-0.7916234708
H7	0.6686084914	-0.3460034986	0.9625355949



H8	-1.8275615536	-0.8030234147	0.0532525179
H9	-2.7861438956	1.6509112477	0.0735467865
H10	-0.7360079622	3.3988984460	0.1159541693
H11	1.5356409318	2.0643799237	0.1231584336

#####mol\_reduced#####

11

structure

C1	0.2680056009	0.1451898849	0.0869583782
C2	-1.2472072348	0.1006053877	0.0710325957
C3	-1.7432640575	1.4125378463	0.0811369464
C4	-0.6655094105	2.3315195412	0.1034817715
C5	0.5514902831	1.6343474600	0.1084085825
H6	0.7353189413	-0.3816190419	-0.7911794131
H7	0.7177100825	-0.4036346842	0.9604955782
H8	-1.8309409688	-0.8144589922	0.0530799682
H9	-2.7955092673	1.6883256834	0.0735643642
H10	-0.7715842727	3.4141215114	0.1150969901
H11	1.5473989551	2.0659658557	0.1234806079

#####mol7#####

#####mol#####

17

structure

C1	-1.5707777792	1.8120707363	0.1021843573
C2	-0.3725212223	1.1150929611	0.0893938478
C3	-0.3629910689	-0.2943295396	0.0900676399
C4	-1.5595666767	-1.0094054318	0.1037757450
C5	-2.7622325863	-0.3027997586	0.1166798951
C6	-2.7702383822	1.0933237164	0.1159028634
C7	1.0327076673	-0.7405382453	0.0746524003
C8	1.8506774644	0.3258703740	0.0648246909
C9	1.0550308343	1.6093210022	0.0731719055
H10	-1.5847540752	2.8973326904	0.1016665249
H11	-1.5589572951	-2.0942108623	0.1043900680
H12	-3.7028677231	-0.8423799346	0.1274207495
H13	-3.7157450393	1.6239370911	0.1260232065
H14	1.3410406623	-1.7785834408	0.0717883904
H15	2.9322897642	0.2987666288	0.0526837361
H16	1.2884693182	2.2275799332	0.9491856805
H17	1.2687968920	2.2269900526	-0.8082339923

#####mol\_reduced#####

17

structure

C1	-1.5569813563	1.8033507999	0.1018224551
C2	-0.3672735726	1.1173529516	0.0896763619
C3	-0.3367228303	-0.3332277006	0.0902171685
C4	-1.5858073540	-1.0205464212	0.1044272670
C5	-2.7725103050	-0.3041240185	0.1168149987
C6	-2.7949431230	1.1079269632	0.1158572224
C7	1.0126924591	-0.7531591784	0.0747255900

C8	1.8784313564	0.3491202789	0.0639394797
C9	1.0680828229	1.6322349435	0.0731962016
H10	-1.5567608736	2.8943312789	0.1009134811
H11	-1.6100134423	-2.1092152058	0.1053528155
H12	-3.7167044335	-0.8481085878	0.1275268237
H13	-3.7360370889	1.6486677205	0.1255940543
H14	1.3299048221	-1.7925776215	0.0715025867
H15	2.9613819925	0.3186183767	0.0516959713
H16	1.2792492707	2.2813650923	0.9482895715
H17	1.2591487605	2.2815758224	-0.8062295576

#####mol\_double\_reduced#####

17

structure

C1	-1.5450730723	1.8005808415	0.0140677524
C2	-0.3611207277	1.1255530787	0.0607664937
C3	-0.3034021327	-0.3491858304	0.1632873778
C4	-1.5976760594	-1.0263442426	0.2513032834
C5	-2.7745682024	-0.2997903430	0.2104617697
C6	-2.8227816995	1.1190527817	0.1272124170
C7	1.0096019732	-0.7358634578	-0.0100079604
C8	1.9180052843	0.3912613281	-0.3485222476
C9	1.0835746729	1.6221107092	0.0951478165
H10	-1.5349389554	2.8959967184	-0.0611144989
H11	-1.6402629778	-2.1155518506	0.3550579580
H12	-3.7239472755	-0.8506269020	0.2669783458
H13	-3.7553982611	1.6299010022	-0.1246906749
H14	1.3222880125	-1.7869456979	-0.0461772375
H15	2.8903381441	0.3447410361	0.1895570696
H16	1.3135959127	1.9554689784	1.1660314615
H17	1.2237276083	2.5383317292	-0.5090999959

#####mol8#####

#####mol#####

16

structure

C1	-0.5702014377	-1.1028556892	0.0891815687
C2	0.8279048626	-0.5659493815	0.0850793093
C3	0.7995755348	0.7900129660	0.1058714341
C4	-0.5904760477	1.2518806328	0.1251714772
C5	-1.3965401869	0.1704191540	0.1160295567
C6	2.1691283365	1.3098847559	0.1021844409
C7	3.0196443318	0.2632271590	0.0795011592
C8	2.2472263206	-1.0436498411	0.0667911266
H9	-0.7852637937	-1.7369848324	0.9597126294
H10	-0.8012541090	-1.7112344602	-0.7954872967
H11	-0.9147281050	2.2844038784	0.1437794022
H12	-2.4782922977	0.1762078253	0.1260789372
H13	2.4500296100	2.3551150707	0.1153708923
H14	4.1002064894	0.3145709140	0.0708014679
H15	2.4889246270	-1.6419276008	-0.8219338043

H16 2.5031055202 -1.6680867517 0.9332611782  
#####mol\_reduced#####

16

structure

C1	-0.5662329158	-1.1204304489	0.0891790346
C2	0.8280559853	-0.5737509528	0.0832806241
C3	0.7987240665	0.8307660570	0.1061745650
C4	-0.5654777248	1.2665103736	0.1255578929
C5	-1.3925591700	0.1642396387	0.1158952912
C6	2.1435458493	1.3234485863	0.1031111678
C7	3.0159344435	0.2568687324	0.0798884791
C8	2.2439908593	-1.0613786341	0.0663293053
H9	-0.7937599429	-1.7848585131	0.9596935755
H10	-0.8115294262	-1.7603891453	-0.7943655410
H11	-0.9061944850	2.2987414500	0.1450739285
H12	-2.4778725816	0.1794148496	0.1266352623
H13	2.4409133761	2.3690837430	0.1168603274
H14	4.0996674160	0.3178390096	0.0715962978
H15	2.5014481479	-1.6904649138	-0.8216556701
H16	2.5133931660	-1.7157060783	0.9324330962

#####mol\_double\_reduced#####

16

structure

C1	-0.4904203093	-1.1043737283	0.0701029457
C2	0.8234413232	-0.5499246089	-0.4350830321
C3	0.7961269206	0.8664442955	-0.0699676928
C4	-0.5306720297	1.2563005776	0.2387434542
C5	-1.3698519238	0.1395404985	0.1436228757
C6	2.1099176720	1.3127687321	0.2170513807
C7	2.9945290801	0.2328754128	0.1074415077
C8	2.1681365777	-1.0475842841	0.0475436378
H9	-0.3160616104	-1.5954626580	1.1404156119
H10	-0.9457025854	-1.9354484512	-0.5081075903
H11	-0.8641235286	2.2733101097	0.4742430558
H12	-2.4128268020	0.1293721229	0.4801582135
H13	2.4033990626	2.3431912086	0.4473265485
H14	4.0422667640	0.2672395624	0.4272566129
H15	2.6487785762	-1.8585954742	-0.5385586269
H16	2.0329660456	-1.5456035750	1.1205283436

#####mol9#####

#####mol#####

24

structure

C1	1.3228352315	-1.8566506139	-0.5388577996
C2	2.3323284714	-1.0922153167	0.0592426886
C3	3.4610388353	-1.7402974927	0.5783893795
C4	3.5630772582	-3.1244372561	0.5313198341
C5	2.5503286170	-3.8791225431	-0.0617328342
C6	1.4369219078	-3.2431451681	-0.6049914639

C7	2.3106254166	0.4089759960	0.0904104487
C8	1.0055894545	1.1502027969	0.1386668206
O9	3.3596646194	1.0300567103	0.0764271694
C10	0.9693188395	2.4448205490	-0.3963612539
C11	-0.1944072484	3.2001647787	-0.3359935521
C12	-1.3310435248	2.6823608373	0.2860384950
C13	-1.2976053563	1.4072729467	0.8448834651
C14	-0.1379677688	0.6399823936	0.7656469557
H15	0.4600237326	-1.3684762437	-0.9744826307
H16	4.2484595310	-1.1361284496	1.0115827860
H17	4.4332379997	-3.6171057982	0.9499273638
H18	2.6327467020	-4.9593174383	-0.1051892500
H19	0.6573233507	-3.8256041164	-1.0825136572
H20	1.8688904979	2.8392868880	-0.8523126255
H21	-0.2166401513	4.1946610780	-0.7668404995
H22	-2.2377840009	3.2743434555	0.3397379222
H23	-2.1734954854	1.0096778071	1.3446971326
H24	-0.1158056627	-0.3456263739	1.2135403368

#####mol\_reduced#####

24

structure

C1	1.2526644050	-1.9769598899	-0.3188089469
C2	2.2968764237	-1.1006146528	0.0771371013
C3	3.5402248282	-1.7135430914	0.3941789528
C4	3.7057970480	-3.0877531934	0.3740509227
C5	2.6497074303	-3.9361233657	0.0130133854
C6	1.4280332392	-3.3545460538	-0.3460562666
C7	2.2455609999	0.3707279201	0.0917568270
C8	0.9804363580	1.1227011970	0.1211900554
O9	3.3400116307	1.0187915386	0.0786088278
C10	1.0344812112	2.5044392233	-0.2107558050
C11	-0.0907869292	3.3099931191	-0.1795096625
C12	-1.3358688497	2.7950716187	0.2080219282
C13	-1.4063093310	1.4478385514	0.5819156103
C14	-0.2829667772	0.6318858136	0.5434741253
H15	0.3081461467	-1.5687429970	-0.6543764731
H16	4.3571078868	-1.0493314506	0.6476822346
H17	4.6712652969	-3.5130756089	0.6391441599
H18	2.7801467508	-5.0135249084	-0.0050013123
H19	0.6037547835	-3.9862264420	-0.6689082094
H20	2.0048470076	2.8991507235	-0.4852072762
H21	-0.0046582175	4.3583175342	-0.4568464916
H22	-2.2178038724	3.4272154548	0.2345338770
H23	-2.3506554853	1.0315761479	0.9249135663
H24	-0.3728270364	-0.3890964962	0.8911598957

#####mol\_double\_reduced#####

24

structure

C1	1.2176474799	-2.0496168432	-0.1737714939
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C2	2.2691254337	-1.0949477868	0.0839201783
C3	3.5743645487	-1.7018898919	0.2521185432
C4	3.7709363376	-3.0668213301	0.2671684646
C5	2.7064572384	-3.9798362468	0.0814047400
C6	1.4332370384	-3.4175310923	-0.1672632368
C7	2.2165982146	0.3535305759	0.0918169243
C8	0.9717482401	1.0955099681	0.1132574716
O9	3.3430354367	1.0208563932	0.0792522566
C10	1.0633658817	2.5302697076	-0.0691829113
C11	-0.0394735977	3.3583392812	-0.0721339756
C12	-1.3480938031	2.8651323425	0.1406847252
C13	-1.4622249384	1.4803797766	0.4028243399
C14	-0.3660346202	0.6342401402	0.3979131558
H15	0.2317176015	-1.6983147594	-0.4510665626
H16	4.3920228250	-0.9996232596	0.3679911097
H17	4.7831366971	-3.4524381683	0.4198402742
H18	2.8645594444	-5.0562441629	0.0915707774
H19	0.5903581386	-4.0770058602	-0.3892915535
H20	2.0698136947	2.9092739917	-0.2055908502
H21	0.1059661447	4.4299663355	-0.2364327535
H22	-2.2164631047	3.5206409748	0.1387531656
H23	-2.4416138621	1.0598786979	0.6449503188
H24	-0.5267551128	-0.3969318703	0.6862946689

#####mol10#####

#####mol#####

24

structure

C1	3.6894734897	-2.6115250056	0.1109002828
C2	2.2993931780	-2.6156965340	0.1156312791
C3	1.5641772376	-1.4214078250	0.1057538270
C4	2.2914757223	-0.2098303398	0.0907419524
C5	3.6906866687	-0.2151794782	0.0860683844
C6	4.3953777741	-1.4087843668	0.0960621941
C7	0.0799162841	-1.4153934801	0.1107278141
C8	-0.6376037629	-0.1979646857	0.1005867977
C9	0.0581101692	1.1132747582	0.0846512171
C10	1.6063152629	1.1070144866	0.0794267177
C11	-0.6648971272	-2.6036782572	0.1255321337
C12	-2.0548993560	-2.5882201513	0.1301136143
C13	-2.7510910604	-1.3797795660	0.1200095968
C14	-2.0368097368	-0.1919458099	0.1052929613
O15	-0.5277747251	2.1727926812	0.0756880230
O16	2.2006555898	2.1617789400	0.0664568563
H17	4.2234121010	-3.5550880666	0.1188749674
H18	1.7916886388	-3.5703461355	0.1272349888
H19	4.1987329334	0.7412071323	0.0744380466
H20	5.4788819980	-1.4067262359	0.0923883394
H21	-0.1648770852	-3.5624053203	0.1337286750
H22	-2.5964263067	-3.5274142315	0.1416624419

H23	-3.8345442690	-1.3689125528	0.1235942372
H24	-2.5371293786	0.7685372687	0.0970665446

#####mol\_reduced#####

24

structure

C1	3.6964872885	-2.6168753299	0.1109440278
C2	2.3122201167	-2.6321569807	0.1157669601
C3	1.5521146739	-1.4440775530	0.1060107556
C4	2.2502478353	-0.2030018588	0.0908101539
C5	3.6613612221	-0.2112387119	0.0861250758
C6	4.3804142687	-1.3888675417	0.0959006118
C7	0.0919182908	-1.4381013180	0.1108861193
C8	-0.5962870528	-0.1914097860	0.1003526735
C9	0.0909897798	1.1153196263	0.0845080827
C10	1.5732269888	1.1091945929	0.0795275739
C11	-0.6777173532	-2.6199546623	0.1257305774
C12	-2.0618205501	-2.5934286869	0.1301905741
C13	-2.7358559410	-1.3599192952	0.1197603585
C14	-2.0073638727	-0.1881843358	0.1051533926
O15	-0.5606478790	2.1795949943	0.0757368691
O16	2.2332359360	2.1681637484	0.0663226991
H17	4.2475357934	-3.5524077865	0.1187952656
H18	1.8078094804	-3.5914359138	0.1274308112
H19	4.1473078281	0.7573744248	0.0744439449
H20	5.4663936871	-1.3688195669	0.0920261724
H21	-0.1810135489	-3.5832822555	0.1339944760
H22	-2.6203733495	-3.5244491179	0.1417253639
H23	-3.8216273913	-1.3310045241	0.1231811059
H24	-2.4853492436	0.7844169480	0.0967427452

#####mol\_double\_reduced#####

24

structure

C1	3.7083955364	-2.6290770349	0.1109766260
C2	2.3261970463	-2.6481944056	0.1158869244
C3	1.5369642266	-1.4713337620	0.1063928287
C4	2.2269476599	-0.1907679841	0.0907903147
C5	3.6514939177	-0.2116770089	0.0861339869
C6	4.3851217801	-1.3743883112	0.0956670907
C7	0.1067478133	-1.4655183858	0.1111844080
C8	-0.5729187024	-0.1794039724	0.1001652032
C9	0.0919560367	1.1176144432	0.0845003578
C10	1.5724669681	1.1116291105	0.0795499153
C11	-0.6919268229	-2.6359179252	0.1260024567
C12	-2.0739255668	-2.6055670760	0.1303555668
C13	-2.7405206577	-1.3454310095	0.1195536366
C14	-1.9975588233	-0.1887287286	0.1050645392
O15	-0.5720999067	2.1995699009	0.0755346224
O16	2.2450921300	2.1882389865	0.0661383966
H17	4.2697605005	-3.5625980345	0.1187376876

H18	1.8263049274	-3.6145994476	0.1276058387
H19	4.1230990351	0.7669271394	0.0743852683
H20	5.4751121574	-1.3409537826	0.0915920834
H21	-0.1998364317	-3.6063549579	0.1343855133
H22	-2.6427794786	-3.5344954632	0.1418990074
H23	-3.8302056675	-1.3031446426	0.1227882521
H24	-2.4612889504	0.7936721880	0.0964499238

#####mol11#####

#####mol#####

23

structure

C1	2.6696956181	1.8740310562	0.0856046689
C2	2.6536945561	0.4816257078	0.0917838026
C3	1.4412663932	-0.2189360790	0.1017391272
C4	0.2326197310	0.5188909879	0.1054060524
C5	0.2625044129	1.9121918620	0.0991567444
C6	1.4761547229	2.5939012336	0.0892618795
C7	1.3775055485	-1.6716748399	0.1083870495
C8	0.2123231942	-2.3839555893	0.1179808888
C9	-1.1007225781	-1.7398620135	0.1226613658
C10	-1.0895460180	-0.1767198657	0.1159072863
O11	-2.1547868765	-2.3379574101	0.1311592525
O12	-2.1413680231	0.4204419717	0.1193037277
C13	0.5019624287	-3.8171635084	0.1222103499
C14	1.8356761232	-3.9889159840	0.1152325297
C15	2.5252996392	-2.6479021592	0.1056745609
H16	3.6186411489	2.3981627556	0.0779133853
H17	3.5902644446	-0.0636927398	0.0888412592
H18	-0.6819421687	2.4429294476	0.1022227370
H19	1.4920562861	3.6772666248	0.0844441728
H20	-0.2595205755	-4.5839371976	0.1297851656
H21	2.3663310176	-4.9308661159	0.1162744152
H22	3.1757999831	-2.5139501995	0.9796623208
H23	3.1661421763	-2.5210014077	-0.7764259395

#####mol\_reduced#####

23

structure

C1	2.6705371618	1.8853069583	0.0854500349
C2	2.6750760796	0.5031505587	0.0915784427
C3	1.4699544432	-0.2381311355	0.1017155035
C4	0.2252076142	0.4757950861	0.1056613767
C5	0.2561888559	1.8820833431	0.0992646846
C6	1.4475304197	2.5853139274	0.0893315083
C7	1.4159736328	-1.6586245159	0.1082898552
C8	0.2078809517	-2.3387113026	0.1178782818
C9	-1.0976449794	-1.7108121172	0.1225422818
C10	-1.0879349767	-0.2063992240	0.1160989038
O11	-2.1584235959	-2.3685592565	0.1312077860
O12	-2.1494848696	0.4439029317	0.1193313155

C13	0.4821001350	-3.7735245861	0.1219933722
C14	1.8113173543	-3.9909424590	0.1152528616
C15	2.5453059012	-2.6657173789	0.1058381571
H16	3.6101388934	2.4305998876	0.0776543561
H17	3.6209237438	-0.0316099438	0.0885755818
H18	-0.7028920136	2.3883145191	0.1024999455
H19	1.4426297184	3.6713345294	0.0845331483
H20	-0.3016656054	-4.5202187833	0.1294498498
H21	2.3106039629	-4.9524847015	0.1164381509
H22	3.2048619567	-2.5594898401	0.9802463962
H23	3.1951518409	-2.5662826230	-0.7765658598

#####mol\_double\_reduced#####

23

structure

C1	2.6792981869	1.8970537421	0.0851076870
C2	2.6978347374	0.5210455335	0.0914817291
C3	1.5004750071	-0.2647323574	0.1019660291
C4	0.2145849223	0.4556130106	0.1058849955
C5	0.2573765406	1.8665648354	0.0991155307
C6	1.4334326131	2.5955492001	0.0890064036
C7	1.4536107488	-1.6486918813	0.1087565702
C8	0.1953206717	-2.3258514697	0.1183896788
C9	-1.1027795187	-1.7139392001	0.1227781386
C10	-1.0902852681	-0.2065284885	0.1161805031
O11	-2.1845431050	-2.3745836968	0.1313111420
O12	-2.1719690828	0.4490711918	0.1192170608
C13	0.4696154989	-3.7446096944	0.1217216744
C14	1.8039757929	-3.9984355694	0.1147031778
C15	2.5710302214	-2.6814494493	0.1059872771
H16	3.6176394141	2.4540051664	0.0770635324
H17	3.6554474517	-0.0010458170	0.0884525804
H18	-0.7129384847	2.3584435930	0.1023615659
H19	1.4143612234	3.6851683951	0.0840383974
H20	-0.3267275913	-4.4833064475	0.1289336007
H21	2.2796891671	-4.9763729676	0.1156788780
H22	3.2474853842	-2.5954350330	0.9802079930
H23	3.2379779362	-2.6010573508	-0.7759244257

#####mol12#####

#####mol#####

16

structure

C1	1.5795634324	-1.5634330435	0.4504217420
C2	0.2295059408	-1.8478274227	-0.0208819234
C3	-0.6249416086	-0.8245843771	-0.2549639477
C4	-0.2114371234	0.5547098328	-0.0417489221
C5	1.1380773584	0.8822555285	0.4319962342
C6	2.0123331453	-0.3028594090	0.6640767032
C7	-1.2715566468	1.3574842818	-0.3577548086
C8	-2.3920384167	0.5158233513	-0.7815245217



C9	-2.0140980079	-0.7875090971	-0.7228600358
O10	1.5454429811	2.0194405898	0.6304474855
H11	2.2437167480	-2.4024505384	0.6297925531
H12	-0.0657828399	-2.8802398775	-0.1758921502
H13	3.0160268831	-0.0926809298	1.0142805754
H14	-1.2806558616	2.4377377191	-0.3035357574
H15	-3.3581449021	0.8906368870	-1.0885280096
H16	-2.6126750027	-1.6522723932	-0.9712940561

#####mol\_reduced#####

16

structure

C1	1.5622722918	-1.5899375488	0.4433260718
C2	0.2538761190	-1.8777694489	-0.0142893477
C3	-0.6227736642	-0.8221608039	-0.2542342153
C4	-0.2061637388	0.5434372860	-0.0406032547
C5	1.1299038313	0.8710046032	0.4285255995
C6	1.9866917670	-0.2932045381	0.6560553185
C7	-1.2914106459	1.3710772452	-0.3635592962
C8	-2.3793401036	0.5457128070	-0.7754335743
C9	-1.9875516426	-0.7869691872	-0.7138942301
O10	1.5446659293	2.0366353208	0.6307838607
H11	2.2480716557	-2.4145545197	0.6309961358
H12	-0.0518615608	-2.9093440358	-0.1727451435
H13	2.9930106648	-0.0813038056	1.0073760435
H14	-1.2900842393	2.4517986831	-0.3056411144
H15	-3.3542506730	0.9057731641	-1.0860173865
H16	-2.5912131774	-1.6522314684	-0.9641553389

#####mol\_double\_reduced#####

16

structure

C1	1.5512048069	-1.6081623489	0.4387006615
C2	0.2743183390	-1.9155563178	-0.0093854304
C3	-0.6311226950	-0.8359672968	-0.2578984348
C4	-0.2014870869	0.5288203042	-0.0398472405
C5	1.1399356327	0.8673996663	0.4316629711
C6	1.9809608497	-0.2769643678	0.6550014357
C7	-1.2959642043	1.3799712197	-0.3645160471
C8	-2.3731608880	0.5695922127	-0.7720051554
C9	-1.9805226335	-0.7936356035	-0.7119298967
O10	1.5282993753	2.0717162782	0.6270637498
H11	2.2577476541	-2.4245893213	0.6339404230
H12	-0.0301252178	-2.9536532351	-0.1676308513
H13	2.9947637428	-0.0721516123	1.0084889074
H14	-1.2767236169	2.4637278812	-0.3002427151
H15	-3.3562362279	0.9297296645	-1.0852531852
H16	-2.5981610715	-1.6556275261	-0.9667636068

#####mol13#####

#####mol#####

16

structure

C1	-2.7198018058	0.6415190000	0.1280813937
C2	-1.5267156111	1.3828525483	0.1149261623
C3	-0.3340110814	0.6925867043	0.0940253248
C4	-0.2925303523	-0.7107245012	0.0858342940
C5	-1.4645724946	-1.4455366204	0.0987261879
C6	-2.6851339257	-0.7487452602	0.1200577805
C7	1.1311323482	-1.1281849667	0.0630812065
C8	1.9333092152	-0.0506015307	0.0573577870
C9	1.0870710087	1.1908883581	0.0762535619
O10	1.4630237976	2.3405676104	0.0770436552
H11	-3.6741673037	1.1547489570	0.1445904304
H12	-1.5353590668	2.4671049249	0.1209146520
H13	-1.4513921286	-2.5300342879	0.0926651777
H14	-3.6154772153	-1.3052795283	0.1304305585
H15	1.4496591586	-2.1632856996	0.0529041191
H16	3.0130511902	-0.0254486856	0.0419502967

#####mol\_reduced#####

16

structure

C1	-2.7105128070	0.6491446487	0.1279827436
C2	-1.5146419062	1.3686510643	0.1146589330
C3	-0.3006668247	0.6885958961	0.0935059611
C4	-0.2720476345	-0.7478065056	0.0853295129
C5	-1.4802529122	-1.4559875465	0.0988948878
C6	-2.6890801212	-0.7599774409	0.1200548679
C7	1.1091353424	-1.1538961873	0.0632540773
C8	1.9068717888	-0.0172420021	0.0579135128
C9	1.0880455783	1.1866634432	0.0762221114
O10	1.4586189398	2.3897909622	0.0774145870
H11	-3.6629999832	1.1725435585	0.1445245237
H12	-1.5123397748	2.4558827896	0.1205051035
H13	-1.4806982690	-2.5449099839	0.0930220635
H14	-3.6267193962	-1.3103798472	0.1305785444
H15	1.4518630457	-2.1829581753	0.0527545322
H16	2.9906338584	0.0111765946	0.0424594888

#####mol\_double\_reduced#####

16

structure

C1	-2.7158622096	0.6567789187	0.1281204927
C2	-1.5009050963	1.3529319378	0.1144034209
C3	-0.2745646635	0.6893671791	0.0931451819
C4	-0.2534847912	-0.7980344397	0.0847978233
C5	-1.4986194705	-1.4745482108	0.0990496679
C6	-2.7016443105	-0.7736751363	0.1201576315
C7	1.0912962766	-1.1837119292	0.0633746076
C8	1.8953402032	0.0134496147	0.0582577240
C9	1.0941722938	1.2031694992	0.0762041021
O10	1.4612464765	2.4456222926	0.0776207566

H11	-3.6667336337	1.1939247601	0.1447166329
H12	-1.4849882216	2.4461099793	0.1201016905
H13	-1.5202914112	-2.5710592657	0.0934332739
H14	-3.6471135613	-1.3233523564	0.1307820450
H15	1.4626441228	-2.2100899584	0.0524939880
H16	2.9878839684	0.0420060131	0.0426875285

#####mol14#####

#####mol#####

17

structure

C1	-1.3973108235	2.0397176371	0.1031066604
C2	-0.1532001758	1.2665165641	0.0897236766
C3	-0.1354871211	-0.0934418420	0.0890625971
C4	-1.3816381734	-0.8933353947	0.1027157348
C5	-2.6487631381	-0.1083706514	0.1166989697
C6	-2.6555148099	1.2316171910	0.1168127127
C7	1.2425599973	-0.5692063497	0.0731874108
C8	2.0613334160	0.5033418386	0.0640373351
C9	1.2555294027	1.7739213632	0.0741267010
O10	-1.3826618222	-2.1114274016	0.1025498106
O11	-1.4310953574	3.2609115565	0.1032768217
H12	-3.5608462324	-0.6950318011	0.1266501480
H13	-3.5754523509	1.8060186336	0.1268721482
H14	1.5247258348	-1.6122670988	0.0696895092
H15	3.1425136175	0.4826598494	0.0515936069
H16	1.4741672412	2.4026749156	0.9466395967
H17	1.4543512238	2.4046117920	-0.8016266390

#####mol\_reduced#####

17

structure

C1	-1.3938295482	2.0578103808	0.1031222459
C2	-0.1855835538	1.2748191295	0.0903895199
C3	-0.1731362894	-0.1103284036	0.0897561150
C4	-1.3802781618	-0.9155712576	0.1027505420
C5	-2.6006837085	-0.1223256903	0.1161076185
C6	-2.6065363197	1.2482887010	0.1162036271
C7	1.2155575743	-0.5617123542	0.0735247955
C8	2.0439670679	0.5034293887	0.0639806230
C9	1.2333820248	1.7806289513	0.0743223404
O10	-1.3764958614	-2.1746883640	0.1023675406
O11	-1.4094778548	3.3195225911	0.1029747467
H12	-3.5318291573	-0.6847948648	0.1260860852
H13	-3.5436792907	1.8009483196	0.1262376065
H14	1.4994513120	-1.6071685136	0.0700476195
H15	3.1273748937	0.4748289010	0.0514217848
H16	1.4500540248	2.4127776869	0.9473600806
H17	1.4297093521	2.4149292493	-0.8018115664

#####mol\_double\_reduced#####

17

structure

C1	-1.3803232291	2.0882130978	0.1030443881
C2	-0.2071717861	1.2919209791	0.0915038898
C3	-0.1955453510	-0.1321804253	0.0908378288
C4	-1.3774828582	-0.9546998975	0.1029742581
C5	-2.5683730645	-0.1392661369	0.1156015025
C6	-2.5663880910	1.2591677942	0.1155215689
C7	1.1858926573	-0.5563038260	0.0737015470
C8	2.0348531460	0.5084817483	0.0633174001
C9	1.2215959701	1.7928133487	0.0744644492
O10	-1.3822964616	-2.2437756156	0.1024503482
O11	-1.3984256346	3.3832434540	0.1024577068
H12	-3.5182471594	-0.6831936426	0.1251812893
H13	-3.5183980001	1.8006532364	0.1249924611
H14	1.4693786390	-1.6068573078	0.0700294577
H15	3.1229000652	0.4659885242	0.0506668771
H16	1.4416316763	2.4402957964	0.9464784421
H17	1.4195486465	2.4427981756	-0.8007527853

#####mol15#####

#####mol#####

17

structure

C1	-3.1213314129	-0.4827344743	0.1165170939
C2	-1.9244531573	-1.1926632842	0.1082249099
C3	-0.7359982720	-0.4670617242	0.0936861645
C4	-0.7431340662	0.9296176769	0.0875671226
C5	-1.9389253362	1.6431595680	0.0958015955
C6	-3.1284959274	0.9211573335	0.1103685944
C7	0.6524119157	1.4553815289	0.0718511645
C8	1.5886348549	0.2431674932	0.0688582140
C9	0.6648685472	-0.9785837504	0.0826069821
O10	0.9778807358	2.6185065998	0.0631624256
O11	1.0023627037	-2.1383042132	0.0842741567
H12	-4.0643306511	-1.0174264737	0.1278882973
H13	-1.9039546212	-2.2760167693	0.1128151532
H14	-1.9294604242	2.7266646137	0.0908935121
H15	-4.0768908240	1.4463008420	0.1170977165
H16	2.2451923321	0.2502940270	0.9433178555
H17	2.2299223416	0.2424552162	-0.8168498985

#####mol\_reduced#####

17

structure

C1	-3.1221869890	-0.4988792800	0.1168387387
C2	-1.9328534615	-1.1939205528	0.1084737940
C3	-0.7098801542	-0.4907353231	0.0935884268
C4	-0.7172191442	0.9534718887	0.0872686469
C5	-1.9473066107	1.6442882497	0.0960021469
C6	-3.1294833069	0.9372666450	0.1105192846
C7	0.6231969917	1.4750332158	0.0719065183

C8	1.5547564373	0.2430475847	0.0693805699
C9	0.6358593649	-0.9985432936	0.0828054244
O10	1.0024401765	2.6579672289	0.0624269929
O11	1.0275301069	-2.1774087832	0.0838435856
H12	-4.0675895753	-1.0345775594	0.1283197225
H13	-1.9160970646	-2.2802460665	0.1131220392
H14	-1.9416700587	2.7307217377	0.0911146144
H15	-4.0802883030	1.4634082084	0.1173226598
H16	2.2149799686	0.2499880968	0.9441522198
H17	2.2008017098	0.2422226038	-0.8158625227

#####mol\_double\_reduced#####

17

structure

C1	-3.1403669416	-0.5170658265	0.1172724309
C2	-1.9465533453	-1.1978696095	0.1087678803
C3	-0.6952813290	-0.5221615528	0.0936305152
C4	-0.7028883314	0.9848424313	0.0871098475
C5	-1.9608856617	1.6479264320	0.0961618374
C6	-3.1477790197	0.9551707799	0.1106835293
C7	0.6013672911	1.5023923279	0.0719181809
C8	1.5244702690	0.2431390526	0.0694262717
C9	0.6142282668	-1.0262463444	0.0828447397
O10	1.0464993352	2.6999600663	0.0618618551
O11	1.0727381576	-2.2186341030	0.0834997221
H12	-4.0889472779	-1.0575432591	0.1288895643
H13	-1.9351719987	-2.2905272865	0.1134905087
H14	-1.9607280252	2.7406208499	0.0912229457
H15	-4.1017557199	1.4861621050	0.1174551512
H16	2.1928248250	0.2494228065	0.9448488517
H17	2.1799268420	0.2419340831	-0.8155958434

#####mol16#####

#####mol#####

17

structure

C1	-0.9280724781	2.4909604566	0.0983364834
C2	0.2064140845	1.7745218423	0.0891477734
C3	0.2123198243	0.2946155449	0.0912333662
C4	-0.9201592293	-0.4446172643	0.1029437286
C5	-2.2222268883	0.2255743037	0.1141115432
C6	-2.2294353369	1.7971715809	0.1114702153
C7	1.6083374554	-0.1200283602	0.0784672221
C8	2.4183767487	0.9527739328	0.0692147381
C9	1.6451550879	2.2493919043	0.0750398415
O10	-3.2802807622	-0.3679978705	0.1250571953
O11	-3.2861035659	2.3883987240	0.1201520224
H12	-0.9482347920	3.5756078053	0.0967751519
H13	-0.9159441402	-1.5287890298	0.1044461254
H14	1.9273493558	-1.1539129632	0.0768034709
H15	3.5004319767	0.9176249623	0.0588736325

H16	1.8810936132	2.8652292136	0.9507648929
H17	1.8645662271	2.8635900413	-0.8060790573

#####mol\_reduced#####

17

structure

C1	-0.9500187071	2.4515544462	0.0987443209
C2	0.2257783801	1.7526261520	0.0890236266
C3	0.2342081831	0.3171136548	0.0910486943
C4	-0.9431023107	-0.4063107312	0.1030505364
C5	-2.2288469523	0.2451103191	0.1139943229
C6	-2.2360587678	1.7755952817	0.1117208444
C7	1.6255421849	-0.1080658483	0.0783838407
C8	2.4608946491	0.9538710768	0.0688578556
C9	1.6631043933	2.2433037633	0.0747278177
O10	-3.3046906606	-0.3891389755	0.1248769921
O11	-3.3088219900	2.4061242815	0.1206619119
H12	-0.9798488248	3.5392989019	0.0973510616
H13	-0.9467100493	-1.4939691401	0.1045928021
H14	1.9366870717	-1.1480857652	0.0769015984
H15	3.5436996922	0.9162754012	0.0587033777
H16	1.8981130407	2.8646576086	0.9506642088
H17	1.8814446266	2.8625832988	-0.8069430533

#####mol\_double\_reduced#####

17

structure

C1	-0.9625785742	2.4303067734	0.0989440860
C2	0.2498339772	1.7392879038	0.0892502618
C3	0.2594727729	0.3282354977	0.0912140439
C4	-0.9675081993	-0.3923306721	0.1034988424
C5	-2.2436705652	0.2356847290	0.1141597683
C6	-2.2426947647	1.7695949773	0.1116835065
C7	1.6377472344	-0.0928160872	0.0782033703
C8	2.5151849627	0.9611482933	0.0679322385
C9	1.6862404029	2.2413334343	0.0746130256
O10	-3.3472017228	-0.3996263839	0.1251947076
O11	-3.3305771635	2.4190038223	0.1204024433
H12	-0.9974006368	3.5245414654	0.0975636282
H13	-0.9682934813	-1.4868379604	0.1049724050
H14	1.9417549477	-1.1419654574	0.0767988302
H15	3.5999576437	0.9195394813	0.0579159743
H16	1.9179283168	2.8705081225	0.9523381305
H17	1.9005789676	2.8688433532	-0.8086157122

#####mol17#####

#####mol#####

11

structure

C1	0.6375952828	-0.3910402006	0.0744772321
C2	-0.5753213344	0.2910073797	0.0743711825
C3	-1.7545653177	-0.4512747167	0.0927495174

N4	-1.7892790448	-1.7871594496	0.1105764893
C5	-0.6167980638	-2.4285674277	0.1104433229
C6	0.6176839547	-1.7823074016	0.0929196114
H7	1.5774479944	0.1496130423	0.0604994095
H8	-0.6113581606	1.3740021785	0.0603936390
H9	-2.7185809032	0.0503369961	0.0931935713
H10	-0.6676100217	-3.5139897918	0.1250925823
H11	1.5359336797	-2.3577955112	0.0937833602

#####mol\_reduced#####

11

structure

C1	0.6873343793	-0.3624996665	0.0737419464
C2	-0.5870436136	0.2961899661	0.0743891349
C3	-1.7489713646	-0.4372558895	0.0925234506
N4	-1.8417656792	-1.8173233774	0.1113551156
C5	-0.6019653548	-2.4307448632	0.1103618159
C6	0.6162633304	-1.7951063600	0.0931000396
H7	1.6269214058	0.1782021976	0.0597626428
H8	-0.6490193878	1.3849583344	0.0605197316
H9	-2.7082402040	0.0879598941	0.0926206698
H10	-0.6299098904	-3.5239434005	0.1249435939
H11	1.5263869817	-2.3960357684	0.0943524833

#####mol\_double\_reduced#####

11

structure

C1	0.7687699066	-0.3167265863	-0.0722187832
C2	-0.6121000017	0.2674295887	-0.1202827724
C3	-1.7419020009	-0.4504429030	0.1597357122
N4	-1.8113609702	-1.7968789459	0.4938498549
C5	-0.6101388599	-2.4173949786	0.1746412182
C6	0.5799256760	-1.8044761227	-0.1049659187
H7	1.3318236591	0.0140042200	0.8668583212
H8	-0.7974745551	1.3065890359	-0.4939425637
H9	-2.7339321983	0.0553447622	0.0152528394
H10	-0.6705794730	-3.5306988347	0.0417630044
H11	1.3883640915	-2.4911024754	-0.4637051935

#####mol18#####

#####mol#####

10

structure

C1	0.5679126536	-1.7793723045	0.0683993429
C2	0.6044178081	-0.3891618509	0.0736437390
C3	-0.6226416206	0.2649894200	0.0954214867
N4	-1.7834739071	-0.3962438588	0.1106800115
C5	-1.6944376915	-1.7282896240	0.1037188776
N6	-0.5799054697	-2.4629622143	0.0833481416
H7	1.4820129319	-2.3667462534	0.0517606384
H8	1.5400836576	0.1559180518	0.0613998732
H9	-0.6824469672	1.3500001658	0.1008797134

H10 -2.6328689198 -2.2749708260 0.1159899102

#####mol\_reduced#####

10

structure

C1	0.6069766861	-1.7767553090	0.0678085626
C2	0.6075899497	-0.3872999912	0.0736065159
C3	-0.6010886289	0.2976505886	0.0952213774
N4	-1.8266220988	-0.3985484258	0.1113242994
C5	-1.6871023930	-1.7239928428	0.1036224750
N6	-0.6031927701	-2.4993708717	0.0835675578
H7	1.5242873973	-2.3595583689	0.0511237293
H8	1.5509974033	0.1624149219	0.0612622376
H9	-0.6553228680	1.3832034549	0.1006042373
H10	-2.6369700443	-2.2773447091	0.1160473667

#####mol\_double\_reduced#####

10

structure

C1	0.6070684899	-1.8071362162	0.0676776020
C2	0.6373480392	-0.3699599817	0.0732167781
C3	-0.6274497125	0.3127718521	0.0956970779
N4	-1.8379830535	-0.3571228412	0.1116821241
C5	-1.7132582490	-1.7392388692	0.1039658858
N6	-0.5727867000	-2.5297333707	0.0829562122
H7	1.5425357308	-2.3914207456	0.0507196731
H8	1.5869895655	0.1833357795	0.0608033664
H9	-0.6740279143	1.4148535052	0.1010237029
H10	-2.6672323619	-2.2950063608	0.1164601875

#####mol19#####

#####mol#####

10

structure

C1	0.8443808443	0.3296758362	0.0732665979
C2	2.0472770638	-0.3484278908	0.0730254779
C3	1.9851595136	-1.7427095874	0.0935370782
N4	0.8444683803	-2.4323637879	0.1129012928
N5	-0.3160698570	-1.7781590056	0.1131239552
C6	-0.3164321228	-0.4451915332	0.0939912988
H7	0.7902182750	1.4117675654	0.0581984824
H8	3.0011255784	0.1654045783	0.0577516553
H9	2.8852908622	-2.3485440004	0.0947544018
H10	-1.3007144360	0.0113719972	0.0955849673

#####mol\_reduced#####

10

structure

C1	0.8246972286	0.3578037733	0.0730311488
C2	2.0814963681	-0.3507113371	0.0727792923
C3	1.9887412272	-1.7352626171	0.0934040789
N4	0.8747507846	-2.4750767745	0.1132448486
N5	-0.3682314601	-1.7743380435	0.1134969902



C6	-0.3118976697	-0.4382123395	0.0938646312
H7	0.7552600764	1.4413413973	0.0580509933
H8	3.0444944024	0.1507789094	0.0576042710
H9	2.9083096070	-2.3312932151	0.0943350531
H10	-1.2978583150	0.0400566714	0.0951691775

#####mol\_double\_reduced#####

10

structure

C1	0.8035977171	0.3928186707	0.0727000129
C2	2.1223759135	-0.3507044466	0.0724592938
C3	1.9983891330	-1.7354414675	0.0933140725
N4	0.9250915912	-2.5317894612	0.1136083490
N5	-0.4428216357	-1.7605519758	0.1139420547
C6	-0.3170212458	-0.4300276064	0.0937987299
H7	0.7127968797	1.4825159808	0.0577529627
H8	3.1017455628	0.1356253522	0.0573925191
H9	2.9535669453	-2.3185433170	0.0937523906
H10	-1.3103622850	0.0854001239	0.0946364518

#####mol20#####

#####mol#####

9

structure

N1	-0.3537333597	-1.7938102872	0.0880213957
C2	-0.3020959473	-0.4605832119	0.0784395375
N3	0.8085068095	0.2788816070	0.0734704973
C4	1.9373465279	-0.4324409822	0.0789642607
N5	2.0224652253	-1.7639477584	0.0885742387
C6	0.8419892326	-2.3858284737	0.0926567580
H7	-1.2496099499	0.0706852424	0.0743059178
H8	2.8712110019	0.1224749701	0.0752816285
H9	0.8556327795	-3.4720131177	0.1004600398

#####mol\_reduced#####

9

structure

N1	-0.3901404187	-1.7819652113	0.0879120761
C2	-0.3089379552	-0.4747320462	0.0785397784
N3	0.8004187149	0.3213207004	0.0731844298
C4	1.9565444281	-0.4482321065	0.0790874338
N5	2.0478268437	-1.7543010374	0.0885002179
C6	0.8504835289	-2.4263079826	0.0929489111
H7	-1.2632743244	0.0664608472	0.0743323401
H8	2.8939191847	0.1146553158	0.0753443072
H9	0.8641773859	-3.5097747164	0.1007542866

#####mol\_double\_reduced#####

9

structure

N1	-0.4061438757	-1.8250155410	0.0882176889
C2	-0.3315582698	-0.4440395848	0.0783112454
N3	0.8077634022	0.3399537527	0.0730374643

C4	1.9664147837	-0.4151719158	0.0788524674
N5	2.0755914313	-1.7937787259	0.0888062107
C6	0.8424183622	-2.4196767134	0.0929001921
H7	-1.2940939327	0.0955852363	0.0741223228
H8	2.9150444519	0.1485320164	0.0751105179
H9	0.8562509388	-3.5230460600	0.1008411171

#####mol21#####

#####mol#####

17

structure

C1	-1.8300636602	-1.2899356119	0.0984987402
C2	-0.5828518924	-0.6156861132	0.0864454084
C3	-0.5625255668	0.8140119044	0.0955891399
C4	-1.7934240896	1.5173084238	0.1165250497
C5	-2.9856050671	0.8353019462	0.1278049214
C6	-3.0057316504	-0.5801230482	0.1187322350
C7	0.6653363387	-1.2836858246	0.0655726507
C8	1.8223399566	-0.5473242812	0.0551398854
C9	1.7301555126	0.8657392142	0.0656218424
N10	0.5967979868	1.5314701744	0.0849738198
H11	-1.8398654045	-2.3751919946	0.0914767957
H12	-1.7528095389	2.5998003079	0.1231364328
H13	-3.9220423431	1.3817252472	0.1438207854
H14	-3.9558018858	-1.1021412129	0.1278663640
H15	0.6910359555	-2.3687969528	0.0581002760
H16	2.7952785594	-1.0240346642	0.0391639575
H17	2.6396356509	1.4625732670	0.0575123766

#####mol\_reduced#####

17

structure

C1	-1.8360504566	-1.2851715236	0.0986180687
C2	-0.5817778996	-0.6272894970	0.0863619022
C3	-0.5583400439	0.8247557091	0.0956140032
C4	-1.7960720007	1.5088843390	0.1165004959
C5	-3.0209047883	0.8223640183	0.1281765249
C6	-3.0419362921	-0.5681110402	0.1192864964
C7	0.6690747295	-1.2959595070	0.0654351169
C8	1.8539050471	-0.5308136039	0.0548124724
C9	1.7630969153	0.8497173824	0.0650850412
N10	0.6029395792	1.5472332451	0.0850131069
H11	-1.8498314692	-2.3734352082	0.0916414895
H12	-1.7589000212	2.5938472256	0.1231660987
H13	-3.9531559140	1.3825766929	0.1442115721
H14	-3.9893430661	-1.1022406844	0.1283004530
H15	0.6981999658	-2.3825332791	0.0579031196
H16	2.8294633984	-1.0112491426	0.0387599783
H17	2.6726625531	1.4531093848	0.0570217181

#####mol\_double\_reduced#####

17

structure

C1	-1.8497617310	-1.2867888733	0.0987815003
C2	-0.5770770583	-0.6428190529	0.0861965621
C3	-0.5545006576	0.8341136586	0.0956284105
C4	-1.8014673063	1.5064867319	0.1165476947
C5	-3.0660152666	0.8158031368	0.1287241161
C6	-3.0847075487	-0.5573210324	0.1199218133
C7	0.6775203888	-1.3025667185	0.0652826163
C8	1.8948335659	-0.5196775406	0.0543368533
C9	1.8011768808	0.8417980940	0.0645350172
N10	0.6137018778	1.5553928610	0.0849428042
H11	-1.8749138829	-2.3809308127	0.0919152252
H12	-1.7662320390	2.5970075949	0.1232701016
H13	-3.9974075811	1.3898566623	0.1448407523
H14	-4.0332005967	-1.1043337007	0.1288783751
H15	0.7155753580	-2.3944149510	0.0576067664
H16	2.8753091523	-1.0071131895	0.0381569330
H17	2.7113328931	1.4579343532	0.0565455449

#####mol22#####

#####mol#####

17

structure

C1	-0.4231787316	-1.2870719786	0.1007980248
C2	0.8203940017	-0.6055264015	0.0860942609
C3	0.8234331714	0.8201286303	0.0920450990
C4	-0.4070781028	1.5218862968	0.1124089827
C5	-1.5961642803	0.8351878310	0.1263227008
C6	-1.6012351878	-0.5808427026	0.1204182811
C7	2.0790167418	-1.2550205977	0.0655907817
C8	3.2268418244	-0.5021794370	0.0525181191
N9	3.2428829586	0.8582965583	0.0579848316
C10	2.0836562388	1.4755729575	0.0769739031
H11	-0.4301527774	-2.3718520215	0.0963341650
H12	-0.3945544995	2.6069086436	0.1168192391
H13	-2.5370773396	1.3730993992	0.1419060015
H14	-2.5481102151	-1.1090409494	0.1315750990
H15	2.1321646383	-2.3383579096	0.0603019997
H16	4.2012748346	-0.9804534643	0.0367444837
H17	2.1088132350	2.5644165052	0.0811923780

#####mol\_reduced#####

17

structure

C1	-0.4253937346	-1.2846057926	0.1008830334
C2	0.8109709848	-0.6145321235	0.0862118982
C3	0.8304034594	0.8321131537	0.0920135489
C4	-0.4179100258	1.5230888630	0.1125593779
C5	-1.6303929759	0.8202738667	0.1267144892
C6	-1.6456723984	-0.5693752413	0.1210906424
C7	2.0872755079	-1.2539875533	0.0654539810

C8	3.2519553395	-0.4878410423	0.0521954316
N9	3.2964060356	0.8458760082	0.0571817539
C10	2.0864195755	1.4727565834	0.0769412583
H11	-0.4318073810	-2.3723386167	0.0964074411
H12	-0.4144588897	2.6103759319	0.1170903646
H13	-2.5684330515	1.3717845943	0.1422763034
H14	-2.5899429628	-1.1075994730	0.1321454039
H15	2.1480693336	-2.3396672417	0.0600122609
H16	4.2196188888	-0.9953953526	0.0363645624
H17	2.1165961502	2.5625304646	0.0810964288

#####mol\_double\_reduced#####

17

structure

C1	-0.4308446966	-1.2821358411	0.1009349081
C2	0.7984692988	-0.6223283225	0.0863284679
C3	0.8412289399	0.8471647194	0.0919105629
C4	-0.4386469112	1.5266828978	0.1128753705
C5	-1.6655390410	0.8096511342	0.1271902960
C6	-1.7031485501	-0.5665082037	0.1219253811
C7	2.1016046152	-1.2541308111	0.0652553371
C8	3.2816386059	-0.4786751166	0.0518390479
N9	3.3610673383	0.8361795472	0.0562344510
C10	2.0926825967	1.4712849447	0.0768337639
H11	-0.4337311860	-2.3768676301	0.0963697513
H12	-0.4523727146	2.6194086733	0.1176807168
H13	-2.6031871858	1.3792972264	0.1428391462
H14	-2.6477891718	-1.1140958373	0.1329745574
H15	2.1748456991	-2.3451281557	0.0596464405
H16	4.2456433910	-1.0199689354	0.0359472400
H17	2.1337953265	2.5656166570	0.0808392937

#####mol23#####

#####mol#####

18

structure

C1	1.8549286464	-0.0092938605	-0.1708582778
C2	0.5082181924	-0.4216657000	-0.2782951861
N3	-0.4785143424	0.3969276225	0.2622636130
C4	-0.1364539082	1.5832256578	0.8871067722
C5	1.1616314359	1.9760190333	0.9880381299
C6	2.1867372665	1.1659026325	0.4487807057
C7	0.1128385882	-1.6231866868	-0.9069901775
C8	-1.2073330836	-1.9783407238	-0.9854877551
C9	-2.1865152541	-1.1256758506	-0.4268175520
C10	-1.8107608594	0.0321333758	0.1796270386
H11	2.6121808154	-0.6553599792	-0.5955404530
H12	-0.9645182453	2.1569518445	1.2780152826
H13	1.3884613186	2.9103337043	1.4839013098
H14	3.2213910519	1.4742676977	0.5266246789
H15	0.8904529298	-2.2503810762	-1.3230987890

H16	-1.5014713528	-2.9009233368	-1.4691992002
H17	-3.2381132038	-1.3756079922	-0.4711692565
H18	-2.5098434937	0.7253406619	0.6250604033

#####mol\_reduced#####

18

structure

C1	1.8613335672	-0.0100185077	-0.1718719656
C2	0.5280568657	-0.4380753448	-0.2891031297
N3	-0.4913528987	0.4074661992	0.2693262514
C4	-0.1301706196	1.6026199778	0.8973322467
C5	1.1577946795	1.9890469314	0.9955496007
C6	2.2091284546	1.1672882455	0.4474911144
C7	0.1140036671	-1.6288419371	-0.9101979244
C8	-1.2075343467	-1.9979742185	-0.9962928201
C9	-2.2016108826	-1.1230072956	-0.4240546697
C10	-1.8324636240	0.0255591183	0.1778868887
H11	2.6208009084	-0.6567956626	-0.5971842106
H12	-0.9560274762	2.1801333800	1.2901921041
H13	1.3867547115	2.9235394365	1.4912953998
H14	3.2423165066	1.4758696764	0.5255406859
H15	0.8925340828	-2.2579793655	-1.3274485770
H16	-1.5019692898	-2.9193105110	-1.4792481566
H17	-3.2532479782	-1.3748522304	-0.4695506013
H18	-2.5357785335	0.7166744368	0.6224595242

#####mol\_double\_reduced#####

18

structure

C1	1.8647286460	-0.0085325255	-0.1713975718
C2	0.5350959643	-0.4439375776	-0.2930698284
N3	-0.4869538078	0.4038988673	0.2668877711
C4	-0.1247346490	1.6068598494	0.8992007128
C5	1.1926249977	2.0048389816	1.0012357771
C6	2.2208067082	1.2064371263	0.4681110068
C7	0.1125523329	-1.6317928089	-0.9117295555
C8	-1.2516214450	-2.0103676683	-0.9991596546
C9	-2.2176967779	-1.1543734284	-0.4398819330
C10	-1.8371139332	0.0206142517	0.1755657451
H11	2.6287068116	-0.6531336081	-0.5958204524
H12	-0.9543522532	2.1810793164	1.2905761964
H13	1.4096301687	2.9446644100	1.5010597271
H14	3.2598798427	1.5090961956	0.5424654837
H15	0.8888293819	-2.2649840062	-1.3310067732
H16	-1.5390399014	-2.9365502478	-1.4853469905
H17	-3.2761109281	-1.3960577292	-0.4790769082
H18	-2.5368946814	0.7152332328	0.6216616475

#####mol24#####

#####mol#####

16

structure

C1	-3.0213436706	-0.5685849056	0.1191715095
C2	-1.8642565241	-1.3053467978	0.0992064956
C3	-0.6067945230	-0.6480371942	0.0865921072
C4	-0.5670651878	0.7761023192	0.0949293747
C5	-1.7798028502	1.5121343293	0.1156526978
C6	-2.9799719390	0.8500888589	0.1274741561
C7	0.6442998999	-1.2919552143	0.0659701737
C8	1.7693724107	-0.5050363101	0.0558937329
N9	1.7420764901	0.8560768796	0.0646833779
N10	0.6019803554	1.4814174987	0.0837523253
H11	-3.9821028308	-1.0705891763	0.1288048486
H12	-1.8944409226	-2.3896953860	0.0928447527
H13	-1.7126336134	2.5930837581	0.1215070109
H14	-3.9094951445	1.4071971845	0.1433144186
H15	0.7162211701	-2.3743868148	0.0582968680
H16	2.7656426660	-0.9310917801	0.0400150492

#####mol\_reduced#####

16

structure

C1	-3.0628262040	-0.5596915753	0.1197665150
C2	-1.8659851979	-1.2940534295	0.0993314740
C3	-0.6151151623	-0.6532710443	0.0866832839
C4	-0.5579351531	0.7904875172	0.0949078301
C5	-1.7886116695	1.5022080550	0.1156855123
C6	-3.0134401588	0.8343640681	0.1277855095
C7	0.6509039431	-1.3015818130	0.0657895190
C8	1.7869394062	-0.4943278447	0.0556991577
N9	1.7981868472	0.8363318343	0.0638528493
N10	0.6019751558	1.4996313031	0.0839099658
H11	-4.0187452433	-1.0762394482	0.1292338710
H12	-1.8941274888	-2.3821155425	0.0929372832
H13	-1.7317788006	2.5859179031	0.1216751592
H14	-3.9373419483	1.4082794331	0.1436205858
H15	0.7281615573	-2.3851787465	0.0579906002
H16	2.7779346941	-0.9516520754	0.0396428199

#####mol\_double\_reduced#####

16

structure

C1	-3.1175420296	-0.5555914737	0.1205310281
C2	-1.8708436490	-1.2888265811	0.0993946823
C3	-0.6244790954	-0.6604895878	0.0867409152
C4	-0.5434700476	0.8100395124	0.0948179516
C5	-1.8081348030	1.5035995214	0.1159666055
C6	-3.0505272312	0.8228308120	0.1282419325
C7	0.6626075982	-1.3064261793	0.0656220310
C8	1.8121931232	-0.4901141685	0.0554187852
N9	1.8678819232	0.8201383050	0.0628168711
N10	0.6019409501	1.5093755285	0.0839350167
H11	-4.0728414345	-1.0838934336	0.1299397485

H12	-1.8961523784	-2.3841094356	0.0929192290
H13	-1.7697783105	2.5931674998	0.1222510951
H14	-3.9735062130	1.4140474500	0.1442111642
H15	0.7510614263	-2.3945432320	0.0576894502
H16	2.8000319926	-0.9856890573	0.0392153545

#####mol25#####

#####mol#####

16

structure

C1	-1.6074885978	-0.5808841374	0.1213416021
C2	-0.4225149754	-1.2801402816	0.1037759327
C3	0.8033307152	-0.5771377513	0.0872438213
C4	0.8011593599	0.8372281275	0.0888964692
C5	-0.4268499456	1.5364108242	0.1070720039
C6	-1.6096659786	0.8334780966	0.1229999390
C7	2.0844587977	-1.1950620210	0.0684142904
N8	3.2236490008	-0.5495644008	0.0530391715
N9	3.2215513312	0.8171716567	0.0546424961
C10	2.0803837694	1.4591257931	0.0715201953
H11	-2.5517608238	-1.1128256908	0.1340907416
H12	-0.4164606786	-2.3646890195	0.1024437673
H13	-0.4241436485	2.6209748554	0.1082847567
H14	-2.5555804454	1.3624645858	0.1369964718
H15	2.1618661734	-2.2799647369	0.0660758094
H16	2.1544554965	2.5442642123	0.0717252496

#####mol\_reduced#####

16

structure

C1	-1.6259367681	-0.6018493318	0.1215774501
C2	-0.4339335205	-1.2833980451	0.1039291111
C3	0.8081613281	-0.6012648238	0.0871466015
C4	0.8060170857	0.8614047263	0.0888601640
C5	-0.4383668751	1.5396681620	0.1072461837
C6	-1.6281009182	0.8543602649	0.1232886740
C7	2.0830036563	-1.1981232753	0.0684338075
N8	3.2496889987	-0.5850915437	0.0526314805
N9	3.2476033379	0.8527500276	0.0543051173
C10	2.0788713748	1.4621703925	0.0715428857
H11	-2.5695249312	-1.1393225816	0.1343049869
H12	-0.4295317151	-2.3734631922	0.1026163319
H13	-0.4373995565	2.6297402910	0.1084883351
H14	-2.5733335493	1.3889257747	0.1372778146
H15	2.1470525232	-2.2914539508	0.0662822557
H16	2.1395549332	2.5556883351	0.0719427186

#####mol\_double\_reduced#####

16

structure

C1	-1.6715663399	-0.5863444968	0.1222357758
C2	-0.4452578973	-1.2879132265	0.1040941841

C3	0.8088023559	-0.6107144862	0.0871367420
C4	0.8065217536	0.8708479283	0.0888743413
C5	-0.4496375827	1.5441074906	0.1074210732
C6	-1.6737669639	0.8387066031	0.1239078513
C7	2.0904448035	-1.1904651012	0.0683353847
N8	3.2952903338	-0.5704270074	0.0519921049
N9	3.2931275967	0.8382546902	0.0536362730
C10	2.0863818599	1.4545610096	0.0714275840
H11	-2.6159103023	-1.1364677964	0.1349551670
H12	-0.4467384438	-2.3829528979	0.1028611916
H13	-0.4544907965	2.6391409020	0.1087556573
H14	-2.6197862025	1.3859135105	0.1379088372
H15	2.1597198115	-2.2892007560	0.0660924822
H16	2.1523016687	2.5535020013	0.0717504573

#####mol26#####

#####mol#####

16

structure

C1	-3.0093834335	-0.5752391652	0.1208250399
C2	-1.8332117783	-1.2837188892	0.1011575139
C3	-0.5968608581	-0.5940930346	0.0867539863
C4	-0.5769607447	0.8291923214	0.0927016248
C5	-1.8048705065	1.5347800162	0.1130937625
C6	-2.9910830025	0.8414562533	0.1267708755
C7	0.6702059307	-1.2268351512	0.0661674458
N8	1.8028677351	-0.5615098040	0.0531545236
C9	1.6986197448	0.7962606826	0.0605655787
N10	0.6014123466	1.5147385828	0.0791288796
H11	-3.9597660648	-1.0958154969	0.1319432067
H12	-1.8356412895	-2.3688028126	0.0964545821
H13	-1.7701734273	2.6172263745	0.1173522461
H14	-3.9311899788	1.3812312133	0.1423952089
H15	0.7313882358	-2.3143458791	0.0605534361
H16	2.6411501532	1.3357983151	0.0496828776

#####mol\_reduced#####

16

structure

C1	-3.0438391506	-0.5618398501	0.1213504737
C2	-1.8426840209	-1.2803058402	0.1013017034
C3	-0.5913510569	-0.6081066972	0.0866330682
C4	-0.5803042366	0.8369194863	0.0928013170
C5	-1.8044753376	1.5237218521	0.1130589122
C6	-3.0312176560	0.8298104952	0.1272803480
C7	0.6700118281	-1.2347478424	0.0661512939
N8	1.8488053421	-0.5419412118	0.0525879969
C9	1.7214430950	0.7787406304	0.0601437513
N10	0.6101305821	1.5277955608	0.0790576740
H11	-3.9909468305	-1.0968311928	0.1323347681
H12	-1.8529354679	-2.3681315415	0.0966851539



H13	-1.7699258417	2.6087731138	0.1173366870
H14	-3.9660984724	1.3843779497	0.1428792605
H15	0.7395898300	-2.3217858753	0.0604266491
H16	2.6576544689	1.3434035028	0.0494232594

#####mol\_double\_reduced#####

16

structure

C1	-3.0782033244	-0.5496604214	0.1218873944
C2	-1.8643532390	-1.2850861688	0.1015881798
C3	-0.5780863569	-0.6280572244	0.0863651219
C4	-0.5882901873	0.8416911628	0.0929454039
C5	-1.8057121785	1.5179445091	0.1130495276
C6	-3.0861792759	0.8281405088	0.1280395053
C7	0.6739818165	-1.2394696546	0.0660682797
N8	1.9064907695	-0.5276035849	0.0518303118
C9	1.7461692638	0.7716279994	0.0597636509
N10	0.6253427042	1.5361727075	0.0788907645
H11	-4.0258091244	-1.1016164244	0.1328011884
H12	-1.8956146472	-2.3780617551	0.0972454024
H13	-1.7634255305	2.6089114060	0.1172336125
H14	-4.0199035684	1.3935537697	0.1436570095
H15	0.7599046250	-2.3296328304	0.0600839383
H16	2.6811138958	1.3632616938	0.0491688035

#####mol27#####

#####mol#####

16

structure

C1	-2.9683118161	-0.5825417016	0.1186977909
C2	-1.7858648415	-1.2809858404	0.1010498842
C3	-0.5521152308	-0.5850373758	0.0883197673
C4	-0.5539975186	0.8435180198	0.0940573050
C5	-1.7895788106	1.5360893649	0.1123577079
C6	-2.9701848368	0.8344228607	0.1243854665
N7	0.6157167831	-1.2855532162	0.0708419627
C8	1.7214467405	-0.5771798228	0.0597874041
C9	1.7195794962	0.8418877750	0.0654907323
N10	0.6119798194	1.5472301447	0.0822234932
H11	-3.9122085245	-1.1157950878	0.1284342924
H12	-1.7559556663	-2.3639413785	0.0963541155
H13	-1.7625129834	2.6191210745	0.1163513062
H14	-3.9154846363	1.3650906318	0.1383926196
H15	2.6631119884	-1.1206039191	0.0457740507
H16	2.6598182571	1.3878616894	0.0558589870

#####mol\_reduced#####

16

structure

C1	-3.0001919514	-0.5711273646	0.1191269217
C2	-1.7874486874	-1.2673351890	0.1011209104
C3	-0.5456375606	-0.5952924506	0.0882104733

C4	-0.5475419852	0.8537903655	0.0940249702
C5	-1.7911130664	1.5224467903	0.1123333543
C6	-3.0020226033	0.8229313055	0.1247339935
N7	0.6189052538	-1.3153420742	0.0707108121
C8	1.7448375119	-0.5577619825	0.0595712005
C9	1.7430305292	0.8225114068	0.0650965914
N10	0.6151002279	1.5770251912	0.0822955150
H11	-3.9390359357	-1.1195903171	0.1287195965
H12	-1.7596872335	-2.3530911547	0.0964356953
H13	-1.7661958745	2.6082735406	0.1163749375
H14	-3.9423077607	1.3688264094	0.1387326086
H15	2.6918296186	-1.0994210886	0.0454984485
H16	2.6885819072	1.3667734484	0.0553640970

#####mol\_double\_reduced#####

16

structure

C1	-3.0428821133	-0.5619885452	0.1197142603
C2	-1.7951894176	-1.2656372152	0.1012276815
C3	-0.5373154723	-0.6101781576	0.0880357954
C4	-0.5392398541	0.8687132182	0.0939834509
C5	-1.7988509309	1.5207253434	0.1124001272
C6	-3.0446787025	0.8136663504	0.1252270790
N7	0.6262064183	-1.3282705750	0.0705318485
C8	1.7799476045	-0.5468253956	0.0591599583
C9	1.7781819739	0.8116720813	0.0646380480
N10	0.6223739934	1.5899720752	0.0822971599
H11	-3.9817109742	-1.1239374854	0.1292796734
H12	-1.7748502461	-2.3571835043	0.0966173051
H13	-1.7814153464	2.6123266306	0.1165367659
H14	-3.9849761064	1.3730630788	0.1392785742
H15	2.7314060374	-1.0971175865	0.0449769314
H16	2.7281926419	1.3645452864	0.0548996915

#####mol28#####

#####mol#####

16

structure

C1	-1.5669445239	-0.5730142237	0.1230177385
C2	-0.4136847713	-1.3133136166	0.1125395484
C3	0.8319947695	-0.6427307846	0.0954748938
C4	0.8267085409	0.7884742158	0.0899376754
N5	-0.3293622607	1.5042141648	0.1005545273
C6	-1.4631060450	0.8397677552	0.1163082833
C7	2.0826047106	-1.3041901047	0.0835592768
C8	3.2303663350	-0.5554936630	0.0673138614
C9	3.1160897041	0.8564892044	0.0631094520
N10	1.9774662373	1.5126350025	0.0737474785
H11	-2.5427692283	-1.0434550043	0.1361697553
H12	-0.4387149217	-2.3984941257	0.1170710817
H13	-2.3699896067	1.4407520939	0.1245009274

H14	2.1156562846	-2.3891548633	0.0874232549
H15	4.2096517433	-1.0187809994	0.0577638900
H16	4.0184934434	1.4640968763	0.0502563642

#####mol\_reduced#####

16

structure

C1	-1.5976030833	-0.5576422159	0.1233261701
C2	-0.4168810048	-1.3192985766	0.1125957009
C3	0.8320520113	-0.6565929784	0.0955210497
C4	0.8266631323	0.8012281059	0.0898810027
N5	-0.3320438905	1.5107445251	0.1005586926
C6	-1.4933094848	0.8234733968	0.1167275169
C7	2.0858489170	-1.3101667239	0.0835418560
C8	3.2609121349	-0.5399057183	0.0669075834
C9	3.1464082971	0.8404090847	0.0628236297
N10	1.9800902423	1.5191901360	0.0736832027
H11	-2.5748322276	-1.0337664500	0.1365294193
H12	-0.4461408629	-2.4064205485	0.1171776586
H13	-2.3978853618	1.4340930225	0.1248521107
H14	2.1231585394	-2.3970402727	0.0873615192
H15	4.2416419765	-1.0088714356	0.0573750341
H16	4.0464457088	1.4576185978	0.0499653109

#####mol\_double\_reduced#####

16

structure

C1	-1.6357877365	-0.5447866697	0.1237183573
C2	-0.4285518126	-1.3273088017	0.1127699431
C3	0.8321242219	-0.6765749701	0.0956031123
C4	0.8266389635	0.8087723395	0.0898560424
N5	-0.3368877518	1.5171397289	0.1005926226
C6	-1.5302829515	0.8169248074	0.1171778234
C7	2.0975775388	-1.3180901281	0.0834308181
C8	3.2989921277	-0.5267678142	0.0664067559
C9	3.1834349969	0.8341320730	0.0624165515
N10	1.9848885750	1.5256267906	0.0736053196
H11	-2.6191141202	-1.0265087942	0.1370061633
H12	-0.4702817103	-2.4197286034	0.1175265405
H13	-2.4344780771	1.4411377915	0.1252311150
H14	2.1474060646	-2.4101744854	0.0871144840
H15	4.2858503021	-1.0013077915	0.0568217076
H16	4.0829898319	1.4649303862	0.0495181215

#####mol29#####

#####mol#####

16

structure

C1	3.1447779877	-0.5892764865	0.1208955353
N2	2.0264532326	-1.2816367240	0.1079555855
C3	0.8571420666	-0.5838596316	0.0941472151
C4	0.8039624894	0.8420285976	0.0932578433

C5	2.0345220561	1.5421171342	0.1075046749
C6	3.2044592546	0.8263156405	0.1213127689
C7	-0.3734175193	-1.2839487714	0.0798913187
C8	-1.5433513308	-0.5681426777	0.0660804881
C9	-1.4836684436	0.8474493056	0.0665051156
N10	-0.3653391574	1.5398046847	0.0794503853
H11	4.0674372980	-1.1649115326	0.1318025638
H12	2.0113610444	2.6255347040	0.1070253319
H13	4.1680764227	1.3222437661	0.1324833874
H14	-0.3502502644	-2.3673664633	0.0803655579
H15	-2.5069745798	-1.0640668920	0.0549023639
H16	-2.4063326599	1.4230677134	0.0555978453

#####mol\_reduced#####

16

structure

C1	3.1765824871	-0.5740186526	0.1212661978
N2	2.0343406324	-1.2919712637	0.1080520710
C3	0.8598809882	-0.5973339046	0.0941835382
C4	0.8012248649	0.8555039100	0.0932192579
C5	2.0331153132	1.5439557059	0.1074872710
C6	3.2342182205	0.8100035626	0.1216701935
C7	-0.3720065516	-1.2857856715	0.0799090377
C8	-1.5731073825	-0.5518350277	0.0657254449
C9	-1.5154753776	0.8321873874	0.0661336201
N10	-0.3732322285	1.5501432327	0.0793534371
H11	4.0986237038	-1.1573381530	0.1321579983
H12	2.0147739529	2.6288288338	0.1070626946
H13	4.1975482052	1.3142038313	0.1328365178
H14	-0.3536670958	-2.3706585536	0.0803325665
H15	-2.5364393213	-1.0560294645	0.0545560764
H16	-2.4375148429	1.4155081845	0.0552423752

#####mol\_double\_reduced#####

16

structure

C1	3.2115869254	-0.5640378013	0.1216748254
N2	2.0502311283	-1.3027288577	0.1082413257
C3	0.8596415446	-0.6112989354	0.0941806579
C4	0.8014726991	0.8694513368	0.0932221053
C5	2.0341775642	1.5477414871	0.1074957512
C6	3.2743272470	0.8010290964	0.1221332157
C7	-0.3730752950	-1.2895702762	0.0798951504
C8	-1.6132285833	-0.5428453482	0.0652534655
C9	-1.5504719315	0.8222255556	0.0657271526
N10	-0.3891167831	1.5608841761	0.0791768054
H11	4.1374017748	-1.1571825323	0.1326159331
H12	2.0209075682	2.6378646911	0.1071283277
H13	4.2413307293	1.3130626535	0.1333374111
H14	-0.3598368152	-2.3796942082	0.0802593834
H15	-2.5802316642	-1.0548741392	0.0540310097

H16 -2.4763010644 1.4153575593 0.0547864793

#####mol30#####

#####mol#####

14

structure

C1	-1.4774474858	-0.5823802417	0.1096525455
N2	-0.3760799465	-1.2949534598	0.1028106572
C3	0.7800825200	-0.5801523068	0.0985775804
C4	0.8003436909	0.8385920175	0.1013314098
N5	-0.3590418303	1.5516251604	0.1084641818
C6	-1.4625585277	0.8421734165	0.1124522678
C7	2.0379015319	-1.2335412331	0.0910886730
N8	3.1681441015	-0.5666063698	0.0868886456
C9	3.0654260044	0.7930233648	0.0901244242
N10	1.9723267826	1.5202813477	0.0969420619
H11	-2.4235235462	-1.1166094055	0.1132188218
H12	-2.4030795715	1.3879830313	0.1181718064
H13	2.0683195137	-2.3204745195	0.0887436680
H14	4.0099484647	1.3284465751	0.0865660889

#####mol\_reduced#####

14

structure

C1	-1.5006459598	-0.5617305272	0.1098059624
N2	-0.3832276609	-1.3189615035	0.1028000106
C3	0.7788351899	-0.5947111628	0.0985558101
C4	0.7912381613	0.8527651385	0.1014138444
N5	-0.3516962633	1.5674209908	0.1084590913
C6	-1.4884194707	0.8203286546	0.1125280067
C7	2.0306307598	-1.2259285906	0.0911363331
N8	3.2047984975	-0.5515524199	0.0867180202
C9	3.0851309718	0.7758281213	0.0899896451
N10	1.9785718130	1.5218351601	0.0969398446
H11	-2.4505163374	-1.0973802514	0.1133890501
H12	-2.4277543423	1.3726260565	0.1182485235
H13	2.0670309790	-2.3133343261	0.0887715158
H14	4.0234558375	1.3337039973	0.0864979622

#####mol\_double\_reduced#####

14

structure

C1	-1.5266787513	-0.5491512047	0.1099532520
N2	-0.4041139153	-1.3365889401	0.1028475796
C3	0.7794166918	-0.6150901750	0.0985068040
C4	0.7804238277	0.8635511892	0.1014846172
N5	-0.3452834502	1.5766156163	0.1084635459
C6	-1.5293888334	0.8126225253	0.1127285025
C7	2.0296329250	-1.2280517300	0.0911499349
N8	3.2543338843	-0.5384830444	0.0865183817
C9	3.1096650739	0.7653831347	0.0898431431
N10	1.9922713347	1.5306067162	0.0968670241

H11	-2.4865871764	-1.0896655300	0.1135591300
H12	-2.4678092130	1.3772894480	0.1184798730
H13	2.0802187217	-2.3192362793	0.0887175628
H14	4.0482663445	1.3467747113	0.0863955185

#####mol31#####

#####mol#####

14

structure

C1	-1.4346454232	-0.5815236160	0.1024094135
N2	-0.3305501743	-1.2894909072	0.0949638245
C3	0.8285676230	-0.5816748989	0.0960010591
C4	0.8271246567	0.8455214539	0.1047138035
N5	-0.3334358781	1.5509290062	0.1123003001
C6	-1.4360941862	0.8406844516	0.1110846445
N7	1.9891168570	-1.2870892087	0.0884113511
C8	3.0917783443	-0.5768569500	0.0896290818
C9	3.0903514522	0.8453462720	0.0983117755
N10	1.9862571805	1.5533135968	0.1057548790
H11	-2.3763155889	-1.1246808726	0.1017690529
H12	-2.3788739089	1.3818861369	0.1170516167
H13	4.0345320591	-1.1180892969	0.0836551562
H14	4.0320271796	1.3884960590	0.0989578661

#####mol\_reduced#####

14

structure

C1	-1.4580306725	-0.5617196628	0.1025947235
N2	-0.3301798111	-1.3011623013	0.0948806949
C3	0.8285872610	-0.5990877632	0.0958892327
C4	0.8271045717	0.8629346324	0.1048167384
N5	-0.3330859564	1.5626056028	0.1123736360
C6	-1.4594423032	0.8208259625	0.1110383864
N7	1.9887769213	-1.2987677140	0.0883455768
C8	3.1151257276	-0.5570083547	0.0896945973
C9	3.1137361957	0.8255363247	0.0981232743
N10	1.9858774326	1.5649922679	0.1058211388
H11	-2.4001714408	-1.1110355203	0.1019192507
H12	-2.4026571281	1.3682502938	0.1170597210
H13	4.0583702784	-1.1043950112	0.0836970195
H14	4.0558397579	1.3749031083	0.0988016034

#####mol\_double\_reduced#####

14

structure

C1	-1.4875992784	-0.5501918159	0.1027514765
N2	-0.3350022234	-1.3157211457	0.0948159246
C3	0.8286065229	-0.6170163078	0.0957855734
C4	0.8270840874	0.8808293022	0.1049264082
N5	-0.3379298515	1.5771542010	0.1124716583
C6	-1.4889857030	0.8092621111	0.1110469478
N7	1.9936306999	-1.3133165234	0.0882419806

C8	3.1446738470	-0.5454242955	0.0896737465
C9	3.1433009147	0.8140302133	0.0979682981
N10	1.9906899283	1.5795470870	0.1058969437
H11	-2.4358067199	-1.1061862058	0.1020467784
H12	-2.4383079152	1.3633086560	0.1171184718
H13	4.0940022333	-1.0994693533	0.0836105650
H14	4.0914989705	1.3700325693	0.0986795120

#####mol32#####

#####mol#####

14

structure

N1	-1.5574581191	-0.5587670977	0.1120618456
C2	-0.4315544915	-1.2337296570	0.1059874892
C3	0.8279400423	-0.5913872684	0.1000333761
C4	0.8273224128	0.8264051187	0.1009011234
N5	-0.3394459280	1.5192290329	0.1071980335
C6	-1.4383503031	0.8003234289	0.1122839945
C7	2.0879957814	-1.2326127333	0.0932836822
N8	3.2133105064	-0.5566582595	0.0880089106
C9	3.0930172057	0.8023241664	0.0894568129
N10	1.9934804632	1.5202617646	0.0954471031
H11	-0.4947465774	-2.3208263462	0.1056431681
H12	-2.3781558312	1.3444468931	0.1173316441
H13	2.1521409763	-2.3196541226	0.0922964298
H14	4.0323477724	1.3472759165	0.0850557257

#####mol\_reduced#####

14

structure

N1	-1.5987669966	-0.5388505953	0.1122990881
C2	-0.4338537770	-1.2372883706	0.1059963947
C3	0.8279495485	-0.6076091095	0.1000149345
C4	0.8273227645	0.8342738726	0.1008897810
N5	-0.3401439298	1.5220431471	0.1071827690
C6	-1.4644891608	0.7811365365	0.1124110216
C7	2.0902882409	-1.2361800523	0.0932689389
N8	3.2546010745	-0.5367127056	0.0878363759
C9	3.1191687388	0.7831504978	0.0893227636
N10	1.9941824160	1.5230737095	0.0954312522
H11	-0.5078042652	-2.3236705037	0.1057077330
H12	-2.3947413674	1.3518002178	0.1174432681
H13	2.1652243692	-2.3224920646	0.0922231463
H14	4.0489200817	1.3546367388	0.0849938301

#####mol\_double\_reduced#####

14

structure

N1	-1.6438151408	-0.5228134434	0.1125222845
C2	-0.4467247309	-1.2441686937	0.1060602964
C3	0.8279641605	-0.6304697460	0.1000029656
C4	0.8273162822	0.8352312756	0.1008983050

N5	-0.3419010618	1.5264835957	0.1072105239
C6	-1.4972076177	0.7740930423	0.1125679113
C7	2.1031544549	-1.2430619233	0.0931949753
N8	3.2996620945	-0.5206297051	0.0876110627
C9	3.1518804726	0.7761340034	0.0891515318
N10	1.9959352875	1.5275256818	0.0954289365
H11	-0.5410612434	-2.3332628978	0.1058808685
H12	-2.4216360952	1.3724729987	0.1175791400
H13	2.1984462708	-2.3320689627	0.0920481663
H14	4.0757698705	1.3753622031	0.0848673468

#####mol33#####

#####mol#####

16

structure

C1	-1.5197788698	1.8227441001	0.0991420363
C2	-0.3382363813	1.0779474244	0.0876550157
C3	-0.3375895322	-0.3437973948	0.0926386489
C4	-1.5681006197	-1.0194702821	0.1096955405
C5	-2.7422960898	-0.2832674516	0.1211165150
C6	-2.7183783059	1.1243867606	0.1158903363
C7	1.0366862133	-0.7602618032	0.0777056358
C8	1.8007353034	0.3734004924	0.0646192157
N9	0.9791792689	1.4848456903	0.0705102705
H10	-1.5043977476	2.9073323678	0.0951522768
H11	-1.5982072320	-2.1036499459	0.1138630283
H12	-3.6971700829	-0.7964358187	0.1343083468
H13	-3.6532364277	1.6731695086	0.1251182048
H14	1.4075340200	-1.7731428369	0.0768339833
H15	2.8734265951	0.4865441552	0.0514341899
H16	1.2961089066	2.4390381260	0.0633745728

#####mol\_reduced#####

16

structure

C1	-1.5119063982	1.8398949098	0.0990007395
C2	-0.3352254675	1.0748720619	0.0876398643
C3	-0.3211317591	-0.3540616304	0.0924830439
C4	-1.5867830057	-1.0440514218	0.1100042185
C5	-2.7656316231	-0.2719093740	0.1213311223
C6	-2.7548829884	1.1179088917	0.1163298826
C7	1.0386458355	-0.7567751889	0.0776844818
C8	1.8524345150	0.3808664739	0.0639729979
N9	0.9817717078	1.4874098740	0.0704768633
H10	-1.4838665856	2.9263998073	0.0948937645
H11	-1.6282026698	-2.1294050279	0.1143312383
H12	-3.7270920514	-0.7863453827	0.1345941686
H13	-3.6933990298	1.6673902518	0.1255962932
H14	1.3983747550	-1.7784288737	0.0769931383
H15	2.9226315843	0.5071132400	0.0507084665
H16	1.2700939117	2.4492893628	0.0636292788



#####mol\_double\_reduced#####

16

structure

C1	-1.5076247840	1.8094832880	0.1744626477
C2	-0.3318855643	1.0818633529	0.1502011193
C3	-0.2982296679	-0.3738176751	0.1080832746
C4	-1.5964349773	-1.0515603178	0.1673475921
C5	-2.7787523931	-0.2861627054	0.1429112065
C6	-2.7972330301	1.1051624559	0.1598958944
C7	1.0238795269	-0.7456796411	-0.0532698613
C8	1.9655742590	0.4070356389	-0.2001454625
N9	0.9959521004	1.5438787389	0.1298970987
H10	-1.4738720449	2.9001688839	0.2582378116
H11	-1.6504600313	-2.1425327316	0.1476748827
H12	-3.7391109525	-0.8200917118	0.1032916664
H13	-3.7318794162	1.6559044953	0.0297812993
H14	1.3603376993	-1.7866176343	-0.1006748473
H15	2.7253077798	0.3786996178	0.6454882253
H16	1.1156656439	2.3458679847	-0.4709086635

#####mol34#####

#####mol#####

16

structure

C1	-1.5593682929	1.8300319417	0.0993214910
C2	-0.3295006675	1.1196601203	0.0872868080
C3	-0.3368402344	-0.3292098735	0.0926793864
C4	-1.5737907596	-1.0270600962	0.1099785875
C5	-2.7394818152	-0.3065915351	0.1212294578
C6	-2.7322633423	1.1214627812	0.1158957773
C7	0.9921935652	-0.7451749937	0.0783638295
N8	1.7630784772	0.3844103464	0.0650588117
C9	1.0037249804	1.5219020740	0.0699485094
H10	-1.5669296932	2.9146690029	0.0954271543
H11	-1.5922742152	-2.1115643446	0.1141790043
H12	-3.6923945000	-0.8242674794	0.1344948600
H13	-3.6798954910	1.6488272200	0.1252519923
H14	1.4338571450	-1.7276364207	0.0766867319
H15	2.7704118571	0.3795276658	0.0530779020
H16	1.4555052054	2.4997185869	0.0609974467

#####mol\_reduced#####

16

structure

C1	-1.5614523838	1.8372923213	0.0993316370
C2	-0.3239032992	1.1281307876	0.0871923521
C3	-0.3313228610	-0.3378065857	0.0926509024
C4	-1.5759764116	-1.0343114115	0.1100226137
C5	-2.7757405770	-0.2906346845	0.1215688077
C6	-2.7686710651	1.1058947937	0.1163703639
C7	0.9969991095	-0.7541051247	0.0783651805

N8	1.8149322782	0.3841883356	0.0644667918
C9	1.0085699879	1.5307990510	0.0698540236
H10	-1.5709008494	2.9247998016	0.0954810964
H11	-1.5964167301	-2.1216663377	0.1142767857
H12	-3.7288498285	-0.8177517502	0.1348432389
H13	-3.7163927495	1.6427220934	0.1256896782
H14	1.4255566669	-1.7455158177	0.0768805284
H15	2.8164322427	0.3791686400	0.0524112080
H16	1.4471943710	2.5177597967	0.0609946308

#####mol\_double\_reduced#####

16

structure

C1	-1.5707748547	1.8282167044	0.0064389243
C2	-0.3328252653	1.1383491650	0.1166730467
C3	-0.3406891255	-0.3462476872	0.1201173113
C4	-1.5861266513	-1.0234600220	0.0133783930
C5	-2.8168562887	-0.2842047997	-0.0148954538
C6	-2.8095547701	1.1021572964	-0.0185528872
C7	0.9888078543	-0.7456103099	0.2877039616
N8	1.9279596635	0.3842353473	0.1886590735
C9	1.0010328947	1.5243870910	0.2835304595
H10	-1.5870763046	2.9231458929	0.0018370556
H11	-1.6141853242	-2.1181438352	0.0139311336
H12	-3.7700399833	-0.8253401587	-0.0191546616
H13	-3.7569061439	1.6533407537	-0.0245804223
H14	1.3870591439	-1.7502741415	0.1349673704
H15	2.3354769009	0.3801111860	-0.8029299068
H16	1.4092436961	2.5237864553	0.1222369634

#####mol35#####

#####mol#####

16

structure

C1	0.3480620646	-1.0070901310	0.0994481121
C2	-0.8883763239	-0.3185788981	0.0868323864
N3	-0.8556427576	1.0962144000	0.0925507973
C4	0.3346588143	1.7872369550	0.1097715151
C5	1.5149634305	1.1121094842	0.1217360480
C6	1.5278338278	-0.3144292847	0.1165398368
C7	-2.1445125974	1.5722699570	0.0785012977
C8	-2.9988843351	0.4847384194	0.0639041923
C9	-2.2281756844	-0.6950071110	0.0689395184
H10	0.3317533409	-2.0902853584	0.0951805350
H11	0.2577575362	2.8662116526	0.1128822536
H12	2.4401789522	1.6728729472	0.1352098942
H13	2.4737096624	-0.8414167209	0.1261830525
H14	-2.3423245422	2.6314543054	0.0800538401
H15	-4.0764543614	0.5452591865	0.0508805435
H16	-2.5920198802	-1.7100482279	0.0606410073

#####mol\_reduced#####

16

structure

C1	0.3444429646	-1.0319165554	0.0993109199
C2	-0.8893386287	-0.3202203141	0.0868217899
N3	-0.8680072241	1.0785935753	0.0923384108
C4	0.3447736613	1.8208477759	0.1100354442
C5	1.5441073162	1.0992792670	0.1220453109
C6	1.5627483477	-0.2926161040	0.1170408962
C7	-2.1575594297	1.5664223343	0.0783078877
C8	-3.0277456480	0.4922111391	0.0635680146
C9	-2.2433156413	-0.6941005505	0.0687631596
H10	0.3282580014	-2.1154014265	0.0950440865
H11	0.2507707386	2.8964898267	0.1129340200
H12	2.4761912320	1.6593106255	0.1355870067
H13	2.5142474306	-0.8181870994	0.1267461984
H14	-2.3401832373	2.6303552706	0.0800566975
H15	-4.1077159703	0.5565583203	0.0505209834
H16	-2.6065274915	-1.7124006874	0.0604674559

#####mol\_double\_reduced#####

16

structure

C1	0.3362663016	-1.0503600412	0.0991020745
C2	-0.8877525086	-0.3361255751	0.0867646617
N3	-0.8876646736	1.0696747884	0.0920516791
C4	0.3662280696	1.8547823102	0.1104178134
C5	1.5743593418	1.0971479770	0.1224123699
C6	1.6154714112	-0.2772071661	0.1177367773
C7	-2.1706875112	1.5587861127	0.0781250117
C8	-3.0677375981	0.5012126382	0.0631552648
C9	-2.2671146566	-0.7016442011	0.0684747937
H10	0.3210182111	-2.1399250026	0.0948118496
H11	0.2606580241	2.9318401801	0.1132147984
H12	2.5136798125	1.6668948024	0.1361180146
H13	2.5752592907	-0.8024199494	0.1275729171
H14	-2.3451023119	2.6296985440	0.0799240657
H15	-4.1516194736	0.5796822065	0.0500597995
H16	-2.6348151150	-1.7247230920	0.0601223409

#####mol36#####

#####mol#####

15

structure

C1	-1.5306192844	1.8558079553	0.1108195013
C2	-0.3376207029	1.1340874083	0.0971976015
C3	-0.3051627253	-0.2795756535	0.0911359164
C4	-1.5026150717	-1.0013670673	0.0988830753
C5	-2.6937782777	-0.2897783826	0.1124470203
C6	-2.7076306759	1.1175413518	0.1183282730
N7	1.0069977925	-0.7328857086	0.0775717328
C8	1.7339132804	0.3493793139	0.0754905178

N9	0.9935189157	1.5100463373	0.0868352070
H10	-1.5470633050	2.9396555080	0.1153989748
H11	-1.4846278618	-2.0843184882	0.0942913039
H12	-3.6364948585	-0.8245707820	0.1186954670
H13	-3.6586626296	1.6374005620	0.1289673748
H14	2.8143574780	0.3739665139	0.0659329644
H15	1.3553034521	2.4495547186	0.0874336963

#####mol\_reduced#####

15

structure

C1	-1.5233938578	1.8712914676	0.1108177422
C2	-0.3341015011	1.1330368070	0.0971637452
C3	-0.2836155208	-0.2925193833	0.0908915993
C4	-1.5182837863	-1.0205079561	0.0989481276
C5	-2.7164126261	-0.2769643733	0.1127017604
C6	-2.7440188244	1.1125740807	0.1186336459
N7	1.0072695067	-0.7380054374	0.0775441513
C8	1.7836868108	0.3542769879	0.0750604201
N9	0.9916776369	1.5170649540	0.0868839710
H10	-1.5279030595	2.9576309435	0.1152992611
H11	-1.5163078692	-2.1049997176	0.0944951340
H12	-3.6641498145	-0.8154850427	0.1189755617
H13	-3.6978293933	1.6344438431	0.1292979821
H14	2.8613526556	0.3859342000	0.0655569248
H15	1.3216550735	2.4662103183	0.0878110738

#####mol\_double\_reduced#####

15

structure

C1	-1.5230846240	1.8404562098	0.0109631516
C2	-0.3279155485	1.1467199921	0.0403809742
C3	-0.2534947433	-0.3103518284	0.1009905182
C4	-1.5279731354	-1.0187252714	0.0914129771
C5	-2.7301430537	-0.2863769740	0.1028024970
C6	-2.7843181840	1.1044315358	0.0544046205
N7	0.9825917523	-0.7528772917	0.2072787667
C8	1.9062041009	0.3633986814	0.3468874123
N9	0.9983081265	1.5947635977	0.0275563734
H10	-1.5268144072	2.9299745879	-0.0931529530
H11	-1.5351210841	-2.1080696217	0.1510263756
H12	-3.6750594553	-0.8436883590	0.1548149053
H13	-3.7353508205	1.6338556205	0.1407716705
H14	2.6223505787	0.2884442943	-0.5296809708
H15	1.1575915109	2.3538993791	0.6741785112

#####mol37#####

#####mol#####

15

structure

C1	-1.5456350240	1.8365457966	0.1059217513
C2	-0.3562152451	1.0949900919	0.0926828591

C3	-0.3509256402	-0.3214181280	0.0927833883
C4	-1.5711768365	-1.0176862666	0.1065279594
C5	-2.7466153361	-0.2901065939	0.1196113702
C6	-2.7305492770	1.1224730901	0.1192740560
C7	1.0347546968	-0.6684213486	0.0773080811
N8	1.8020948798	0.4025532471	0.0685972931
N9	0.9588193296	1.4664164363	0.0779173356
H10	-1.5415212703	2.9202432709	0.1057561308
H11	-1.5900200183	-2.1014984564	0.1068622985
H12	-3.6997021273	-0.8056930762	0.1303511400
H13	-3.6721997170	1.6595159616	0.1297681034
H14	1.4841835032	-1.6502294309	0.0723829954
H15	1.3473022986	2.3942357397	0.0734620751

#####mol\_reduced#####

15

structure

C1	-1.5381842011	1.8472869383	0.1058446054
C2	-0.3578483498	1.0956986264	0.0927048559
C3	-0.3333184591	-0.3342586485	0.0925944878
C4	-1.5862540503	-1.0382685254	0.1067049592
C5	-2.7708744919	-0.2783694584	0.1198809162
C6	-2.7709202882	1.1131852899	0.1197279073
C7	1.0338898924	-0.6657408818	0.0773169198
N8	1.8593923026	0.4114790733	0.0679389571
N9	0.9591817460	1.4719634109	0.0779090453
H10	-1.5234035895	2.9333898691	0.1055567330
H11	-1.6177525368	-2.1235042528	0.1071779173
H12	-3.7275224363	-0.8004250722	0.1306494025
H13	-3.7143142098	1.6534237773	0.1302335380
H14	1.4726642643	-1.6563946539	0.0725158426
H15	1.3176681188	2.4095444794	0.0737913895

#####mol\_double\_reduced#####

15

structure

C1	-1.5351966033	1.8584056025	0.1057762837
C2	-0.3580250787	1.0999924340	0.0926974248
C3	-0.3148797393	-0.3465167354	0.0923898453
C4	-1.6112107236	-1.0581751280	0.1069526803
C5	-2.7978488398	-0.2740857031	0.1201820272
C6	-2.8235027851	1.1099623360	0.1203207913
C7	1.0403559963	-0.6644858139	0.0772739935
N8	1.9310171221	0.4153068182	0.0671664832
N9	0.9638940147	1.4811102708	0.0778633993
H10	-1.5086790002	2.9508940678	0.1053235633
H11	-1.6588559641	-2.1481201293	0.1075614440
H12	-3.7608004435	-0.8072723324	0.1310550146
H13	-3.7729719204	1.6515347404	0.1309672005
H14	1.4678620191	-1.6695148074	0.0725965093
H15	1.2945492265	2.4301300275	0.0740438530

#####mol38#####

#####mol#####

15

structure

N1	1.7024094792	1.8021652486	0.0993488278
C2	0.6191976637	1.0341131771	0.0958853959
C3	0.5734991853	-0.3889425435	0.0988954214
C4	1.8061808919	-1.0494699586	0.1063356891
C5	2.9554693520	-0.2695800699	0.1100887834
C6	2.8562984183	1.1320901050	0.1064231805
C7	-0.8113485123	-0.7603335102	0.0930534961
C8	-1.5345737119	0.4023182909	0.0869231885
N9	-0.6787307433	1.4865168541	0.0885965107
H10	1.8655486239	-2.1323321114	0.1090853377
H11	3.9361667203	-0.7297039372	0.1158541379
H12	3.7576973113	1.7376895139	0.1093769715
H13	-1.2212094106	-1.7579141852	0.0933363280
H14	-2.6031660593	0.5487050942	0.0814272917
H15	-0.9376456948	2.4591743609	0.0851304878

#####mol\_reduced#####

15

structure

N1	1.6909460986	1.8365209671	0.0992141125
C2	0.6195874707	1.0283374129	0.0958911339
C3	0.5639847270	-0.3949340647	0.0988597064
C4	1.8265565745	-1.0860874405	0.1065142936
C5	2.9729765313	-0.2588127141	0.1101536402
C6	2.8809002093	1.1235757084	0.1065659125
C7	-0.8108018949	-0.7548838197	0.0930430273
C8	-1.5785762111	0.4087374247	0.0867098519
N9	-0.6818341223	1.4821830557	0.0885847800
H10	1.8955088865	-2.1687343945	0.1093057237
H11	3.9653922098	-0.7091521179	0.1159610304
H12	3.7862016771	1.7291110413	0.1095460722
H13	-1.2108331174	-1.7615314843	0.0933896235
H14	-2.6451309393	0.5655545222	0.0812179408
H15	-0.9092782246	2.4611995735	0.0852483410

#####mol\_double\_reduced#####

15

structure

N1	1.7094882503	1.8467814801	0.0992672736
C2	0.5997111828	1.0365577144	0.0957704131
C3	0.5691093720	-0.3894706292	0.0988690237
C4	1.8311875428	-1.1009971945	0.1065749548
C5	2.9849631194	-0.2695010022	0.1102437219
C6	2.8783186336	1.1155355717	0.1065706150
C7	-0.8136539169	-0.7565399628	0.0930262014
C8	-1.5570539101	0.4163413633	0.0868023988
N9	-0.7028913428	1.4789731542	0.0884989707

H10	1.8958759085	-2.1875149320	0.1093681074
H11	3.9873677079	-0.7110285869	0.1160855649
H12	3.7986285112	1.7130009056	0.1096410632
H13	-1.2274158995	-1.7701227093	0.0933134953
H14	-2.6404457378	0.6372003593	0.0810913647
H15	-1.1109872971	2.5037231732	0.0841967670

#####mol39#####

#####mol#####

14

structure

C1	0.3324019817	-0.9237087199	0.1010251568
C2	-0.9104284807	-0.2474140225	0.0971514969
N3	-0.8712601469	1.1571615539	0.1003692893
C4	0.3344828004	1.8164856301	0.1069833236
C5	1.4716992575	1.0658846272	0.1102496802
N6	1.4868082034	-0.3024261109	0.1073462380
C7	-2.1743543540	1.5826748289	0.0957019644
C8	-2.9328662051	0.4249554155	0.0899221081
N9	-2.1615679323	-0.6921680497	0.0908083306
H10	0.3258672013	-2.0095161413	0.0986290373
H11	0.3165915979	2.8975917254	0.1092605157
H12	2.4368102493	1.5576916283	0.1154745191
H13	-2.4403757613	2.6260245538	0.0968307971
H14	-4.0109530503	0.3604540342	0.0851464309

#####mol\_reduced#####

14

structure

C1	0.3226586368	-0.9369856042	0.1009484646
C2	-0.9112617628	-0.2519224477	0.0971398921
N3	-0.8859140337	1.1430109154	0.1002806195
C4	0.3488601371	1.8370369611	0.1070981368
C5	1.4926074048	1.0523955341	0.1103090385
N6	1.5429717861	-0.2818868737	0.1076218092
C7	-2.1944380607	1.5798116309	0.0956031974
C8	-2.9588877655	0.4347662683	0.0898338953
N9	-2.1835483842	-0.6980273340	0.0907089965
H10	0.3244924141	-2.0205535128	0.0985943955
H11	0.3217692777	2.9169684656	0.1093329163
H12	2.4539382175	1.5721235676	0.1155748350
H13	-2.4488077139	2.6280672167	0.0967779748
H14	-4.0400347253	0.3732388276	0.0850483307

#####mol\_double\_reduced#####

14

structure

C1	0.3101419831	-0.9482482099	0.1008758421
C2	-0.9103368614	-0.2652655582	0.0971158077
N3	-0.9075769517	1.1392780928	0.1001766290
C4	0.3712222981	1.8610438870	0.1072521860
C5	1.5190083814	1.0458115385	0.1104094655

N6	1.6120006171	-0.2655333418	0.1079520162
C7	-2.2131930592	1.5756687010	0.0955032071
C8	-2.9959595167	0.4420285201	0.0896963821
N9	-2.2145883399	-0.7113943826	0.0905400916
H10	0.3254569926	-2.0355313753	0.0985738797
H11	0.3463112253	2.9447320091	0.1095216351
H12	2.4816043626	1.5983885902	0.1157532773
H13	-2.4631793154	2.6308879447	0.0967108301
H14	-4.0835481372	0.3901202626	0.0849219037

#####mol40#####

#####mol#####

13

structure

C1	1.7847481029	1.8113483784	0.1176979254
C2	0.5648766021	1.1494983994	0.1034579881
C3	0.5619219310	-0.2661217469	0.0849574602
N4	1.6871544768	-0.9816756222	0.0807650645
C5	2.7977917454	-0.2478324725	0.0954584640
N6	2.9080034689	1.0944298429	0.1135006651
N7	-0.7341144989	-0.7447905657	0.0727742762
C8	-1.4787308818	0.3285202947	0.0833783957
N9	-0.7683630851	1.5065009909	0.1020080632
H10	1.8778311956	2.8943601038	0.1322679148
H11	3.7353103635	-0.7945174847	0.0926334816
H12	-2.5595363121	0.3294410051	0.0784417595
H13	-1.1531850066	2.4374181320	0.1123982058

#####mol\_reduced#####

13

structure

C1	1.7742715575	1.8337698471	0.1179405758
C2	0.5628812842	1.1480919837	0.1034330150
C3	0.5434385357	-0.2728416484	0.0847876025
N4	1.7053998103	-1.0080112263	0.0805080985
C5	2.8073389451	-0.2319534162	0.0957102235
N6	2.9481251082	1.0876116020	0.1135916948
N7	-0.7333405918	-0.7457330577	0.0727615159
C8	-1.5252504897	0.3286155687	0.0831649714
N9	-0.7680701872	1.5113085621	0.1020762647
H10	1.8626946967	2.9165584819	0.1324780826
H11	3.7487882022	-0.7900030968	0.0927496642
H12	-2.6035414196	0.3355190456	0.0783075865
H13	-1.1245118714	2.4511621623	0.1127154564

#####mol\_double\_reduced#####

13

structure

C1	1.7664000356	1.8072770422	0.0076856446
C2	0.5567784768	1.1615619765	0.0191248478
C3	0.5133716866	-0.2921978377	0.0879528006
N4	1.7216058461	-1.0155305719	0.0842026948



C5	2.8148792721	-0.2371701691	0.0914413519
N6	2.9882971424	1.0785987828	0.0721069471
N7	-0.7054381436	-0.7568537441	0.2107391280
C8	-1.6406835551	0.3365395966	0.3536487871
N9	-0.7718487447	1.5873387183	0.0000431085
H10	1.8570139180	2.8950892305	-0.0642709078
H11	3.7621508570	-0.8087843936	0.1250601903
H12	-2.3852553014	0.2361498515	-0.4880686312
H13	-0.9492573261	2.3608023728	0.6254743108

#####mol41#####

#####mol#####

21

structure

C1	0.9925537494	2.2409844083	-0.1304949569
C2	-0.1814018873	1.5160779142	0.1264564080
N3	-1.3495821879	2.1379163356	0.3608447010
C4	-1.3757271345	3.4698544256	0.3675779335
C5	-0.2556964073	4.2667251479	0.1452456916
C6	0.9528778077	3.6287797442	-0.1153391996
C7	-0.2051673977	0.0289280321	0.1322911245
C8	-1.4172640834	-0.6458753480	-0.0699597193
C9	-1.4639270845	-2.0348439967	-0.0792750332
C10	-0.3025827100	-2.7790676167	0.1227976393
C11	0.9056915810	-2.1208118168	0.3388732271
C12	0.9541135768	-0.7300952836	0.3433499399
H13	1.9166914101	1.7266461863	-0.3597701576
H14	-2.3433739433	3.9245014734	0.5632476748
H15	-0.3347796674	5.3467644229	0.1675714204
H16	1.8510528647	4.2030356523	-0.3134701890
H17	-2.3139430697	-0.0579163217	-0.2145050312
H18	-2.4094718254	-2.5392065586	-0.2445588153
H19	-0.3398251060	-3.8625658262	0.1175718171
H20	1.8118514685	-2.6902604296	0.5126422635
H21	1.8992986494	-0.2377264147	0.5392567400

#####mol\_reduced#####

21

structure

C1	1.0278092442	2.2676094113	0.1252622723
C2	-0.1778793116	1.4920106876	0.1257801175
N3	-1.4011340280	2.1573691088	0.1198020058
C4	-1.4010669214	3.4798235837	0.1157274218
C5	-0.2691018851	4.3022049105	0.1168707109
C6	0.9855414659	3.6403101505	0.1209623394
C7	-0.1951473829	0.0563813934	0.1313660032
C8	-1.4356260201	-0.6626512301	0.1296056684
C9	-1.4808466724	-2.0425394311	0.1347271888
C10	-0.3061843151	-2.8194771866	0.1427527364
C11	0.9233469424	-2.1380723631	0.1456591586
C12	0.9854552538	-0.7562368220	0.1402483674

H13	1.9902844142	1.7677760170	0.1289191148
H14	-2.3912252889	3.9456290424	0.1107803048
H15	-0.3575335165	5.3828562505	0.1115458550
H16	1.9113443344	4.2115514323	0.1212555784
H17	-2.3458123563	-0.0767927134	0.1235712167
H18	-2.4503137448	-2.5380293486	0.1333311860
H19	-0.3474364584	-3.9038784419	0.1476425802
H20	1.8520738863	-2.7060528648	0.1515123372
H21	1.9633564616	-0.2865446081	0.1423462413

#####mol\_double\_reduced#####

21

structure

C1	1.0296506273	2.2776653996	-0.0186154584
C2	-0.1939197267	1.4742501604	0.0627942390
N3	-1.4359422905	2.2030739680	0.0070227957
C4	-1.3903194260	3.5043727464	0.1587805932
C5	-0.2464961112	4.3202675314	0.3445075720
C6	1.0026835353	3.6358679429	0.1175946085
C7	-0.2112232033	0.0840530714	0.1305343843
C8	-1.4560820073	-0.6956672589	0.1079524653
C9	-1.4739889328	-2.0690479183	0.0963278993
C10	-0.2877503372	-2.8629194261	0.1186944167
C11	0.9305846105	-2.1385826271	0.2161944285
C12	0.9885251466	-0.7622061248	0.2269376885
H13	1.9722052376	1.7830422794	-0.2533180089
H14	-2.3726653902	4.0100082770	0.1201595863
H15	-0.3276091629	5.4064209216	0.3178185048
H16	1.9316211421	4.2064234125	0.0116430220
H17	-2.3819477383	-0.1299078890	0.0877928429
H18	-2.4466899588	-2.5734108184	0.0719786935
H19	-0.3184081628	-3.9502722640	0.1470428290
H20	1.8715659143	-2.6939525647	0.3022690313
H21	1.9592336024	-0.2859412085	0.3519891753

#####mol42#####

#####mol#####

21

structure

C1	0.4529236363	2.4855096388	0.4906669329
C2	0.3726005921	1.1560500538	0.0599547267
C3	1.5612483564	0.5731814918	-0.4067806995
N4	2.7404637380	1.1939027620	-0.4529478530
C5	2.7877442808	2.4608964049	-0.0313211797
C6	1.6730743380	3.1481933955	0.4428018738
C7	-0.8996494052	0.3958720939	0.0861030910
C8	-2.1094572532	1.0061423827	-0.2752385457
C9	-3.3042104179	0.2935637990	-0.2507789735
C10	-3.3143752391	-1.0457752327	0.1333060628
C11	-2.1198189349	-1.6654170396	0.4939258483
C12	-0.9252362294	-0.9521461699	0.4719945816

H13	-0.4278385449	2.9859103409	0.8774826631
H14	1.5491070558	-0.4473509693	-0.7795845920
H15	3.7593983297	2.9449013580	-0.0746481430
H16	1.7630815518	4.1755420089	0.7758828934
H17	-2.1106678318	2.0409259903	-0.5991030221
H18	-4.2273924384	0.7832763703	-0.5399181022
H19	-4.2449110217	-1.6014558141	0.1513867953
H20	-2.1179108691	-2.7052618043	0.8009356623
H21	-0.0060913345	-1.4385535200	0.7777071258

#####mol\_reduced#####

21

structure

C1	0.4239077942	2.5813587721	0.1388604897
C2	0.3560343851	1.1438890826	0.0622980340
C3	1.6436402517	0.5165887661	-0.0284067884
N4	2.8166360502	1.1224797530	-0.0447721276
C5	2.8328490633	2.4821640450	0.0347221369
C6	1.6479385020	3.2218013891	0.1262039572
C7	-0.8760659609	0.4041395916	0.0665823645
C8	-2.1582191377	1.0493679572	-0.0104236708
C9	-3.3455291692	0.3407868978	-0.0027831831
C10	-3.3680184596	-1.0611959382	0.0856531331
C11	-2.1266455454	-1.7226519122	0.1647351607
C12	-0.9332567156	-1.0282478915	0.1555992560
H13	-0.4814626569	3.1686226187	0.2381352654
H14	1.6938080031	-0.5675017851	-0.1101006467
H15	3.8078609966	2.9619203263	0.0172144150
H16	1.6938967272	4.3073302548	0.1932673818
H17	-2.2052663095	2.1281677077	-0.1066005781
H18	-4.2833412709	0.8891144423	-0.0736472462
H19	-4.3025927867	-1.6119071503	0.0949160564
H20	-2.1005497480	-2.8079005836	0.2431724216
H21	-0.0127250638	-1.5939930562	0.2422812985

#####mol\_double\_reduced#####

21

structure

C1	0.4316849863	2.6064556417	0.1949856597
C2	0.3393753842	1.1332247257	0.1251112628
C3	1.6734168468	0.5221303561	0.2190832479
N4	2.8322039647	1.1244072690	0.0736774475
C5	2.8392073671	2.4867077042	-0.1552305100
C6	1.6459781765	3.2287638785	0.0244802692
C7	-0.8512831368	0.4138144594	0.0341782124
C8	-2.1769913419	1.0525760599	-0.0415179182
C9	-3.3535295721	0.3428144951	0.0299629258
C10	-3.3958027804	-1.0737304078	0.1571898432
C11	-2.1340557147	-1.7327617675	0.0753850527
C12	-0.9401071971	-1.0552296569	-0.0012741785
H13	-0.4456670356	3.1939089810	0.4630425033

H14	1.7339920317	-0.5431899467	0.4634655393
H15	3.8148880531	2.9704622840	-0.2182382683
H16	1.7022041087	4.3234321720	0.0789894056
H17	-2.2236823759	2.1264890560	-0.2136222083
H18	-4.2967145106	0.8969820960	-0.0416772617
H19	-4.3335175479	-1.6233276040	0.2019512429
H20	-2.1094288178	-2.8278790474	0.0392028433
H21	-0.0255714413	-1.6311867651	-0.1289838110

#####mol43#####

#####mol#####

21

structure

C1	0.8983538099	-0.7281411704	0.4774343061
C2	-0.2447819364	-0.0112520313	0.0961791223
C3	-1.3836996595	-0.7305971518	-0.2929579477
C4	-1.3782644777	-2.1216083144	-0.3029657619
C5	-0.2365843822	-2.8209822170	0.0808990396
C6	0.9010390131	-2.1191907015	0.4723274290
C7	-0.2490995587	1.4721031409	0.1042907329
C8	0.8672837364	2.2138762921	-0.3009927827
C9	0.8120041417	3.6034529166	-0.2748440141
N10	-0.2572651935	4.3012328929	0.1197412084
C11	-1.3224973575	3.5930166264	0.5066183165
C12	-1.3697660855	2.2029360547	0.5175827858
H13	1.7801037366	-0.1905720530	0.8067037870
H14	-2.2685713421	-0.1946327202	-0.6164035617
H15	-2.2648327158	-2.6598398570	-0.6184966314
H16	-0.2334397594	-3.9047419890	0.0750322729
H17	1.7907448665	-2.6556373501	0.7820170886
H18	1.7610621503	1.7169855138	-0.6591489152
H19	1.6712422273	4.1867570938	-0.5945651092
H20	-2.1850615468	4.1678568111	0.8326573546
H21	-2.2606603079	1.6970196329	0.8702377872

#####mol\_reduced#####

21

structure

C1	0.9662648996	-0.7627284347	0.0917756029
C2	-0.2448001539	0.0104071137	0.0980820698
C3	-1.4513742190	-0.7698772603	0.0943813122
C4	-1.4399478778	-2.1511591044	0.0852552092
C5	-0.2363067206	-2.8792165061	0.0788390405
C6	0.9629969454	-2.1440020830	0.0823311187
C7	-0.2490009480	1.4441317018	0.1060119405
C8	0.9421838516	2.2486734015	0.1009871422
C9	0.8764607321	3.6243501947	0.1072817732
N10	-0.2575286561	4.3684488850	0.1181058259
C11	-1.3870871375	3.6177854294	0.1231785024
C12	-1.4448706646	2.2417453280	0.1182978497
H13	1.9224195095	-0.2522486499	0.0944019714

H14	-2.4105590755	-0.2650757300	0.0983694548
H15	-2.3892146735	-2.6836371621	0.0826104559
H16	-0.2331050221	-3.9638692279	0.0715295462
H17	1.9153599800	-2.6708631061	0.0778818414
H18	1.9228378406	1.7862338039	0.0914155655
H19	1.8072539958	4.1943142393	0.1021599173
H20	-2.3211190099	4.1822924389	0.1328049264
H21	-2.4228367363	1.7735894975	0.1239498967

#####mol\_double\_reduced#####

21

structure

C1	0.9799280338	-0.7924906731	0.0925919684
C2	-0.2448963445	0.0307464997	0.0975480933
C3	-1.4649304273	-0.7996048217	0.0983880753
C4	-1.4414053680	-2.1741821527	0.0859126793
C5	-0.2363164802	-2.9333432940	0.0752966644
C6	0.9643521462	-2.1672026856	0.0814834026
C7	-0.2489892448	1.4217856442	0.1012600138
C8	0.9512953197	2.2775818357	0.0990082296
C9	0.8749897982	3.6455285259	0.1102655425
N10	-0.2575365713	4.4261718590	0.1259977222
C11	-1.3856424264	3.6389696933	0.1238303480
C12	-1.4540868679	2.2706116311	0.1114465544
H13	1.9447795264	-0.2901013824	0.1007666208
H14	-2.4326817848	-0.3028547092	0.1081406845
H15	-2.4003150269	-2.7046755435	0.0872494850
H16	-0.2332598051	-4.0208087479	0.0635804881
H17	1.9263200093	-2.6921084598	0.0776057851
H18	1.9412766143	1.8252135642	0.0833902474
H19	1.8177451981	4.2111573361	0.1078976647
H20	-2.3316910275	4.1990046766	0.1307046068
H21	-2.4415175538	1.8123834972	0.1096348362

#####mol44#####

#####mol#####

20

structure

C1	0.9978094183	2.1731712954	0.0798938076
C2	-0.2233869469	1.4883870428	0.0977599598
N3	-1.4041112401	2.1263509807	0.1125040398
C4	-1.4003070049	3.4588615172	0.1098659892
C5	-0.2375894148	4.2258803782	0.0926404591
C6	0.9856206823	3.5614561447	0.0773721974
C7	-0.2606709811	-0.0015257133	0.1011818528
N8	0.9200548328	-0.6394898586	0.0864661323
C9	0.9162491353	-1.9720008714	0.0891484692
C10	-0.2464701974	-2.7390224444	0.1063914220
C11	-1.4696754350	-2.0745971340	0.1216101826
C12	-1.4818617431	-0.6863154393	0.1190344236
H13	1.9163246132	1.6030639630	0.0685533216

H14	-2.3753995552	3.9384404353	0.1221342503
H15	-0.2951695681	5.3076578989	0.0913248683
H16	1.9165426100	4.1173097842	0.0636910437
H17	1.8913414907	-2.4515787342	0.0768995944
H18	-0.1888910179	-3.8207972324	0.1077500712
H19	-2.4005949260	-2.6304535520	0.1352976991
H20	-2.4003790799	-0.1162075796	0.1303300955

#####mol\_reduced#####

20

structure

C1	1.0009608128	2.1881496873	0.0798561143
C2	-0.2305403628	1.4597624804	0.0979355108
N3	-1.4353551483	2.1425596077	0.1128993193
C4	-1.4004892338	3.4670163268	0.1098328929
C5	-0.2441233301	4.2529210763	0.0926500066
C6	0.9926586912	3.5610862843	0.0772774223
C7	-0.2535762469	0.0270978448	0.1010431689
N8	0.9512585711	-0.6556576616	0.0860717945
C9	0.9164614402	-1.9801094769	0.0891375413
C10	-0.2398728777	-2.7660616423	0.1063311304
C11	-1.4766809157	-2.0742724640	0.1217097074
C12	-1.4850480162	-0.7013366215	0.1191293575
H13	1.9218827814	1.6189894253	0.0685106900
H14	-2.3764728473	3.9604307545	0.1220701710
H15	-0.3033085693	5.3358394766	0.0913311993
H16	1.9308415398	4.1118324110	0.0635038924
H17	1.8924687450	-2.4734801128	0.0768872614
H18	-0.1806345375	-3.8489784950	0.1076479992
H19	-2.4148402898	-2.6250575219	0.1354883040
H20	-2.4059904769	-0.1322166526	0.1304796515

#####mol\_double\_reduced#####

20

structure

C1	1.0087983647	2.2111632990	0.0797329902
C2	-0.2338682503	1.4383966187	0.0980446250
N3	-1.4669551219	2.1723923720	0.1132990928
C4	-1.4014614402	3.4856790830	0.1098066991
C5	-0.2481752136	4.2965470035	0.0925807056
C6	0.9994204289	3.5749595496	0.0771553721
C7	-0.2502253509	0.0484872939	0.1009649394
N8	0.9828497429	-0.6855202585	0.0856877545
C9	0.9174177092	-1.9987914006	0.0891385006
C10	-0.2358561651	-2.8097024047	0.1063510496
C11	-1.4834332873	-2.0881281332	0.1218279200
C12	-1.4928497210	-0.7243254909	0.1192872560
H13	1.9360090066	1.6466330805	0.0683254041
H14	-2.3814138672	3.9966372316	0.1220643762
H15	-0.3103880863	5.3824731656	0.0912628798
H16	1.9480834604	4.1211277010	0.0632554508

H17	1.8973796617	-2.5097404348	0.0768545293
H18	-0.1735577711	-3.8956207511	0.1076231827
H19	-2.4321309731	-2.6342294940	0.1357352508
H20	-2.4201165565	-0.1598868148	0.1307318353

#####mol45#####

#####mol#####

20

structure

C1	-1.3974093516	2.2295995468	-0.1881442491
C2	-0.2501636985	1.4580722841	0.0427434716
C3	0.9508243958	2.1487295547	0.2427526221
C4	0.9450723324	3.5361037632	0.2309506166
C5	-0.2615795139	4.1979938215	0.0122769415
N6	-1.4174278379	3.5633546535	-0.2028751900
C7	-0.2765688452	-0.0265938963	0.0580725398
N8	0.8958108037	-0.6457269000	-0.1601738934
C9	0.9240257328	-1.9778402066	-0.1575098926
C10	-0.1985152973	-2.7735266317	0.0579532861
C11	-1.4109230022	-2.1364126976	0.3010008724
C12	-1.4532159231	-0.7482475328	0.3077500166
H13	-2.3490574710	1.7486212806	-0.3951125899
H14	1.8592089989	1.5816831176	0.3988362978
H15	1.8566236263	4.1000841563	0.3898848645
H16	-0.3034666081	5.2835361970	0.0043457646
H17	1.8937573060	-2.4331959144	-0.3394051727
H18	-0.1178124852	-3.8534098920	0.0432473668
H19	-2.3101971546	-2.7108989169	0.4922546137
H20	-2.3797687168	-0.2324024618	0.5228517452

#####mol\_reduced#####

20

structure

C1	-1.4276796858	2.2554716111	0.0493803027
C2	-0.2562478401	1.4326766623	0.0430220433
C3	0.9777376762	2.1626983027	0.0298311736
C4	0.9609973018	3.5428464778	0.0270414699
C5	-0.2599212285	4.2322083937	0.0359969375
N6	-1.4481530460	3.5785649331	0.0464361409
C7	-0.2793891582	-0.0014711080	0.0474588031
N8	0.9444293599	-0.6613771402	0.0330204933
C9	0.9461638954	-1.9857358172	0.0352641553
C10	-0.1841462698	-2.8066470256	0.0510799143
C11	-1.4397988289	-2.1477708897	0.0683570220
C12	-1.4843364670	-0.7750290439	0.0666298255
H13	-2.4099455082	1.7859969702	0.0575787794
H14	1.9017749607	1.5996025118	0.0231212468
H15	1.8947254723	4.1019180482	0.0172959341
H16	-0.3008941190	5.3186327760	0.0329727500
H17	1.9365221417	-2.4499091562	0.0237777945
H18	-0.0948327146	-3.8871435828	0.0532147712

H19	-2.3641242737	-2.7204835740	0.0832525515
H20	-2.4462383830	-0.2747905510	0.0804948551

#####mol\_double\_reduced#####

20

structure

C1	-1.4370575615	2.2770085480	0.0334171440
C2	-0.2507154668	1.4111731373	0.0422825424
C3	0.9952627710	2.1941074035	0.0308874828
C4	0.9565706963	3.5666741463	0.0323581381
C5	-0.2698946255	4.2778120931	0.0405205280
N6	-1.4608852500	3.5931614136	0.0342041023
C7	-0.2728778809	0.0178980849	0.0549730640
N8	0.9791530324	-0.6978292792	0.0495172100
C9	0.9431335277	-2.0109289424	0.0334304196
C10	-0.1895627012	-2.8508860358	0.0305342931
C11	-1.4531200999	-2.1575996168	0.0686288991
C12	-1.4903197310	-0.7928453245	0.0822968604
H13	-2.4232432645	1.8037601986	0.0215395655
H14	1.9311460123	1.6467353215	0.0223389331
H15	1.8963809321	4.1309497492	0.0253837029
H16	-0.3176831965	5.3669838881	0.0362442119
H17	1.9347819424	-2.4992387391	0.0262501680
H18	-0.1025832655	-3.9348393307	0.0158983903
H19	-2.3903910014	-2.7211321924	0.0965272846
H20	-2.4554982315	-0.2915580399	0.1246178908

#####mol46#####

#####mol#####

20

structure

C1	-1.4548518809	2.2050495984	-0.1059503376
C2	-0.2937602017	1.4440249835	0.0674956151
C3	0.9046669091	2.1461505123	0.2349749973
C4	0.8830965182	3.5358925434	0.2359016128
N5	-0.2259982593	4.2670718286	0.0776075451
C6	-1.3665653202	3.5936954866	-0.0936446731
C7	-0.2988151166	-0.0436628603	0.0725890361
N8	0.8833742963	-0.6440486561	-0.1413059817
C9	0.9307242136	-1.9750113538	-0.1486817510
C10	-0.1819511284	-2.7877733466	0.0566094545
C11	-1.4050281478	-2.1700493832	0.2938295894
C12	-1.4669455465	-0.7823376018	0.3049322104
H13	-2.4181079335	1.7390452329	-0.2728297888
H14	1.8302248015	1.6002600970	0.3576912934
H15	1.8058017509	4.0935408807	0.3711230679
H16	-2.2609495041	4.1950279041	-0.2326140211
H17	1.9079031607	-2.4150014471	-0.3284001695
H18	-0.0857820466	-3.8664850528	0.0378508496
H19	-2.2974833128	-2.7584591638	0.4743098934
H20	-2.4041730382	-0.2819067812	0.5101465910



#####mol\_reduced#####

20

structure

C1	-1.4752561964	2.2263111685	0.0739317302
C2	-0.2975117386	1.4117910640	0.0703393069
C3	0.9181436754	2.1680879402	0.0600149026
C4	0.8891164305	3.5447831686	0.0557385126
N5	-0.2282745842	4.3149238585	0.0592266913
C6	-1.3781777163	3.6026435899	0.0674814759
C7	-0.2958221550	-0.0197345481	0.0743118984
N8	0.9321564692	-0.6672452393	0.0639978909
C9	0.9489085034	-1.9898301009	0.0656448022
C10	-0.1755390605	-2.8226618223	0.0778867814
C11	-1.4352333018	-2.1774068132	0.0916846313
C12	-1.4945715208	-0.8049361451	0.0895364967
H13	-2.4644986715	1.7807929296	0.0785884079
H14	1.8589101114	1.6327632175	0.0561927008
H15	1.8314711739	4.0945514384	0.0481790010
H16	-2.2947582298	4.1951749436	0.0704681071
H17	1.9435455878	-2.4441563662	0.0581592081
H18	-0.0756571926	-3.9022301182	0.0805982526
H19	-2.3534322164	-2.7601421010	0.1052508930
H20	-2.4604883947	-0.3126399702	0.1026489084

#####mol\_double\_reduced#####

20

structure

C1	-1.4829532473	2.2491261491	0.0646381103
C2	-0.2930778287	1.3856600010	0.0693964936
C3	0.9267706954	2.2022711039	0.0602935316
C4	0.8807107321	3.5701902417	0.0594308426
N5	-0.2387406719	4.3743382989	0.0633020408
C6	-1.3815273186	3.6176994583	0.0618112247
C7	-0.2881985964	-0.0018752821	0.0796092325
N8	0.9672573412	-0.7062058257	0.0749322349
C9	0.9458104937	-2.0183338241	0.0618118729
C10	-0.1798200608	-2.8705936868	0.0601971887
C11	-1.4468611903	-2.1907635500	0.0914232248
C12	-1.5009450983	-0.8268537319	0.1024093755
H13	-2.4806775451	1.8123570603	0.0542137677
H14	1.8812885533	1.6856226694	0.0550630108
H15	1.8327765233	4.1190138380	0.0537408315
H16	-2.3145220247	4.1997031063	0.0576024203
H17	1.9421909399	-2.4962148620	0.0558687695
H18	-0.0822777456	-3.9535307476	0.0471144581
H19	-2.3779074197	-2.7653367605	0.1141821342
H20	-2.4705332956	-0.3335441458	0.1388946780

#####mol47#####

#####mol#####

20

structure

C1	0.4718467116	2.4593813621	0.4731126456
C2	0.4003990030	1.1133678096	0.0972238057
C3	1.5983667932	0.4983444969	-0.2832728915
C4	2.7769674328	1.2375341169	-0.2716645826
N5	2.8472525940	2.5224681474	0.0881466255
C6	1.7026268509	3.1077237594	0.4525341589
C7	-0.8844542118	0.3734937322	0.1018907534
C8	-2.0816506385	0.9822913634	-0.2908600706
C9	-3.2602762007	0.2433541172	-0.2697136990
N10	-3.3312843057	-1.0356261836	0.1105951286
C11	-2.1873969484	-1.6149224286	0.4866462317
C12	-0.9566553521	-0.9662991688	0.4992545720
H13	-0.4128763427	2.9919262293	0.8007306034
H14	1.6131359905	-0.5352061482	-0.6076749087
H15	3.7123969542	0.7735352483	-0.5719607156
H16	1.7724399776	4.1506200597	0.7491641417
H17	-2.0957527858	2.0104920970	-0.6318681035
H18	-4.1951022189	0.7024250084	-0.5793121316
H19	-2.2578298572	-2.6529138805	0.7998821297
H20	-0.0725880258	-1.4934799578	0.8371684025

#####mol\_reduced#####

20

structure

C1	0.4704559616	2.5320870380	0.0879281414
C2	0.3775736545	1.1003280023	0.0961423163
C3	1.6624983759	0.4619418130	0.1005576268
C4	2.8245343222	1.2023777748	0.0958552137
N5	2.9033033874	2.5546650494	0.0886590798
C6	1.6941746230	3.1653815694	0.0852701457
C7	-0.8616951464	0.3866522577	0.1007573515
C8	-2.1466989808	1.0248736986	0.0924093933
C9	-3.3086474329	0.2842954546	0.0975438217
N10	-3.3872660867	-1.0679399641	0.1120688463
C11	-2.1780740446	-1.6784769334	0.1208457854
C12	-0.9544335324	-1.0450566970	0.1154686859
H13	-0.4249476359	3.1433015828	0.0852040619
H14	1.7416611281	-0.6192929011	0.1055060777
H15	3.7822645358	0.6799086929	0.0996549799
H16	1.7230773971	4.2559614209	0.0787937359
H17	-2.2259935261	2.1060314480	0.0799385950
H18	-4.2664350159	0.8066387745	0.0911302949
H19	-2.2067925798	-2.7690274008	0.1320107247
H20	-0.0589497880	-1.6561042609	0.1245426395

#####mol\_double\_reduced#####

20

structure

C1	0.4942598464	2.5558636526	0.0879740015
C2	0.3585002256	1.0892850197	0.0971947390

C3	1.6951375048	0.4705278393	0.1040585026
C4	2.8444816653	1.2165054307	0.0968506851
N5	2.9572940603	2.5857084803	0.0845947526
C6	1.7164018460	3.1754143407	0.0822245098
C7	-0.8425177887	0.3975639609	0.0996601221
C8	-2.1791919772	1.0163023765	0.0919403964
C9	-3.3285080008	0.2703048140	0.1002791676
N10	-3.4413294746	-1.0988583910	0.1163416656
C11	-2.2004825181	-1.6885252264	0.1199643632
C12	-0.9783171957	-1.0689784020	0.1122870851
H13	-0.3961105314	3.1820384251	0.0867718794
H14	1.7898250076	-0.6138020295	0.1158347009
H15	3.8039315283	0.6806446224	0.1034746669
H16	1.7344992786	4.2742163877	0.0753809674
H17	-2.2739050666	2.1005871254	0.0776055166
H18	-4.2879634984	0.8061696884	0.0945955121
H19	-2.2183238169	-2.7873216205	0.1293091835
H20	-0.0879606918	-1.6951830852	0.1150185963

#####mol48#####

#####mol#####

28

structure

C1	-2.1015441072	-1.1586919677	0.1311268649
C2	-0.7213835916	-1.1899446298	0.1308432576
C3	0.0059032218	0.0019845690	0.0003956414
C4	-0.7150200106	1.1947140655	-0.1293640639
C5	-2.0981875227	1.1698692881	-0.1300918852
N6	-2.7722468932	0.0083207610	0.0001875986
C7	1.4941310114	-0.0017676801	-0.0004476547
C8	2.2215164405	0.9652943663	0.7082503419
C9	3.6016789261	0.9378709013	0.6928807388
N10	4.2722464543	-0.0074154110	-0.0040011588
C11	3.5980603233	-0.9481435148	-0.6975940642
C12	2.2148716683	-0.9697597885	-0.7094379668
C13	5.7636606084	0.0047035159	0.0053149517
C14	-4.2636713932	-0.0070557490	0.0023303179
H15	-2.7016764533	-2.0529842909	0.2392797485
H16	-0.2304753999	-2.1461620838	0.2576278383
H17	-0.2211041657	2.1493383312	-0.2562479311
H18	-2.6904022358	2.0685289324	-0.2381674743
H19	1.7306903215	1.7300059883	1.2962104305
H20	4.2018929801	1.6583499553	1.2334790190
H21	4.1902039523	-1.6723773302	-1.2406038401
H22	1.7207992610	-1.7331108809	-1.2964190164
H23	6.1274115733	-0.8200747050	-0.6014724163
H24	6.1110777725	0.9502649002	-0.4099957317
H25	6.1106289093	-0.1105235802	1.0317543199
H26	-4.6276273674	1.0106177979	-0.1100742255
H27	-4.6111181351	-0.6177912437	-0.8304730340

H28 -4.6104803568 -0.4211555549 0.9486284216  
#####mol\_reduced#####

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structure

C1	-2.1035334516	-1.1289539717	-0.3094506411
C2	-0.7417306651	-1.1567146693	-0.3157029064
C3	0.0349121105	0.0021576617	0.0015557704
C4	-0.7368197486	1.1630302523	0.3191761197
C5	-2.1001469434	1.1404782883	0.3126955850
N6	-2.8012338694	0.0084308213	0.0015308912
C7	1.4651054894	-0.0021060117	0.0001918646
C8	2.2420127351	1.1600613419	0.3040695921
C9	3.6037005202	1.1324480465	0.2954708522
N10	4.3012084435	-0.0082687888	-0.0035529438
C11	3.5999432575	-1.1442040179	-0.2996529046
C12	2.2365555998	-1.1665304527	-0.3051243356
C13	5.7704394727	0.0083117220	0.0032569355
C14	-4.2704529128	-0.0094174026	-0.0017141489
H15	-2.6991667594	-1.9991854651	-0.5492676358
H16	-0.2733371142	-2.0950553402	-0.5743046691
H17	-0.2661141233	2.1000403200	0.5777556312
H18	-2.6896477141	2.0141079991	0.5530023187
H19	1.7740249624	2.1021902499	0.5489316101
H20	4.1994493209	2.0060519223	0.5223480137
H21	4.1892755874	-2.0211286078	-0.5280788104
H22	1.7654486711	-2.1072952609	-0.5492494361
H23	6.1395933159	-0.9770526766	-0.2718864137
H24	6.1393521482	0.7393818139	-0.7180697137
H25	6.1380078638	0.2599251579	0.9995972398
H26	-4.6397432331	0.9805722993	0.2560976148
H27	-4.6389332091	-0.2784045907	-0.9930659578
H28	-4.6382668935	-0.7281143812	0.7326349651

#####mol\_double\_reduced#####

28

structure

C1	-2.1029665591	-1.1398654050	-0.3024177036
C2	-0.7541442948	-1.1673654050	-0.3109467360
C3	0.0589626571	0.0026604989	0.0002393217
C4	-0.7504916042	1.1768144329	0.3127633766
C5	-2.0993850027	1.1528802106	0.3062017223
N6	-2.8250466894	0.0084369339	0.0028975028
C7	1.4411550124	-0.0033248817	0.0020304544
C8	2.2541999700	1.1654232367	0.3180226454
C9	3.6029700840	1.1381417680	0.3086213045
N10	4.3249406378	-0.0079627063	-0.0044843888
C11	3.5994014422	-1.1514848571	-0.3111617444
C12	2.2505899566	-1.1763833966	-0.3143278717
C13	5.7729288644	0.0131212168	-0.0003906556
C14	-4.2730774397	-0.0117674236	-0.0045657128

H15	-2.6986833879	-2.0139224240	-0.5339020930
H16	-0.2855009973	-2.1098155296	-0.5598910730
H17	-0.2798371769	2.1184452304	0.5603182701
H18	-2.6909458402	2.0294476440	0.5377565871
H19	1.7855670081	2.1052051222	0.5767598144
H20	4.1986888457	2.0104983261	0.5462139285
H21	4.1910227544	-2.0265016947	-0.5480840047
H22	1.7798458787	-2.1163891044	-0.5678370676
H23	6.1473358314	-0.9754700355	-0.2659415343
H24	6.1676456598	0.7323399383	-0.7284209557
H25	6.1693219052	0.2715431622	0.9891598112
H26	-4.6475120523	0.9768429850	0.2610209991
H27	-4.6676200283	-0.2693582244	-0.9951354711
H28	-4.6695585844	-0.7312892298	0.7222147846

#####mol49#####

#####mol#####

23

structure

C1	3.5548919577	-1.7571999168	0.0828200095
N2	2.2337162922	-1.7711945672	0.0948070055
C3	1.5763056311	-0.5900993809	0.0991410963
C4	2.2589568512	0.6570284137	0.0912249143
C5	3.6673194493	0.6302002545	0.0785359116
C6	4.3244221014	-0.5801925888	0.0742533000
C7	0.1251735650	-0.6067889014	0.1123518756
C8	-0.5811031725	0.6263052927	0.1169952590
C9	0.1505248268	1.8605136942	0.1085999677
C10	1.5083076321	1.8775538808	0.0962929860
C11	-0.5995657612	-1.8151986052	0.1206776959
C12	-1.9794136535	-1.8066539226	0.1332381246
C13	-2.6823028623	-0.5879226724	0.1378910142
C14	-1.9931630260	0.6064238809	0.1298889365
H15	4.0453628887	-2.7274682578	0.0796963658
H16	4.2186605166	1.5650137544	0.0722633515
H17	5.4062743753	-0.6365485441	0.0645481572
H18	-0.4083284086	2.7905584018	0.1123381685
H19	2.0487194086	2.8185505275	0.0900802016
H20	-0.0420665725	-2.7425006533	0.1169248317
H21	-2.5252190667	-2.7433708192	0.1395601809
H22	-3.7664756706	-0.5887573296	0.1477802511
H23	-2.5302621426	1.5492439053	0.1334400681

#####mol\_reduced#####

23

structure

C1	3.5890277527	-1.7673338427	0.0825398334
N2	2.2289754516	-1.7785831712	0.0948932245
C3	1.5849581289	-0.5982155064	0.0990952704
C4	2.2683115274	0.6702028290	0.0911142861
C5	3.6939029581	0.6329206530	0.0782312560

C6	4.3430159681	-0.6078625340	0.0740796534
C7	0.1258130760	-0.5932516839	0.1123504118
C8	-0.5953977518	0.6594084351	0.1171165589
C9	0.1187515129	1.8689952294	0.1089323597
C10	1.5137768306	1.8688569734	0.0962767759
C11	-0.6026514488	-1.7978587188	0.1206931341
C12	-1.9854371086	-1.8190292004	0.1332840390
C13	-2.6984251373	-0.5925971043	0.1379885235
C14	-2.0219303103	0.6024161818	0.1301374498
H15	4.0704615764	-2.7436689494	0.0795368270
H16	4.2548602948	1.5629275422	0.0718359873
H17	5.4288899151	-0.6672900733	0.0643153448
H18	-0.4290865868	2.8079695643	0.1125716274
H19	2.0539786930	2.8132513833	0.0900437152
H20	-0.0257930245	-2.7156589142	0.1167763424
H21	-2.5222729645	-2.7626453018	0.1395309940
H22	-3.7857282570	-0.5991524600	0.1478762472
H23	-2.5728096410	1.5406422847	0.1337983390

#####mol\_double\_reduced#####

23

structure

C1	3.5943632764	-1.7637389517	0.0825005850
N2	2.2470114408	-1.7979327374	0.0947817134
C3	1.5705549359	-0.5852977135	0.0992110036
C4	2.2858146420	0.6884312155	0.0909185535
C5	3.7105020696	0.6483559893	0.0780553774
C6	4.3690308879	-0.6071958848	0.0738468457
C7	0.1364486814	-0.5959158207	0.1122535003
C8	-0.6066019591	0.6582958511	0.1172281405
C9	0.1249698247	1.8679574118	0.1088677746
C10	1.5354322538	1.8786988707	0.0960402343
C11	-0.6160126371	-1.8162173663	0.1208185621
C12	-2.0222400763	-1.8165295083	0.1335977107
C13	-2.7363354401	-0.6175956821	0.1383840548
C14	-2.0312553823	0.6106691618	0.1302343378
H15	4.0917901278	-2.7423533854	0.0793593668
H16	4.2715017385	1.5837288909	0.0716518857
H17	5.4585207351	-0.6773898256	0.0640618881
H18	-0.4261635131	2.8106109028	0.1125319451
H19	2.0711644642	2.8310885547	0.0898187271
H20	-0.0528299007	-2.7420369119	0.1170117784
H21	-2.5584931468	-2.7686681143	0.1398227772
H22	-3.8280856736	-0.6217896534	0.1483132490
H23	-2.5787385625	1.5550116383	0.1338685537

#####mol50#####

#####mol#####

23

structure

N1	3.6738532259	-1.7749045573	0.0790120266
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C2	2.3518524290	-1.7631457122	0.0911475876
C3	1.5527685580	-0.5967836451	0.0978856200
C4	2.2382781539	0.6465629851	0.0909448525
C5	3.6473667751	0.6254171151	0.0780255718
C6	4.3074924556	-0.5830508553	0.0725839938
C7	0.0992280491	-0.6172785264	0.1112739513
C8	-0.6006958616	0.6226853522	0.1170766355
C9	0.1362290106	1.8532543195	0.1096340932
C10	1.4927297595	1.8698609810	0.0971491487
C11	-0.6590152648	-1.8084948278	0.1188876538
C12	-2.0389986496	-1.7785690456	0.1316249155
C13	-2.7249869737	-0.5526518589	0.1373266328
C14	-2.0123207296	0.6265938124	0.1301162401
H15	1.8824852400	-2.7417378634	0.0959657617
H16	4.2033571266	1.5566066571	0.0724385812
H17	5.3925535713	-0.6229215489	0.0626500797
H18	-0.4217709923	2.7839323548	0.1142726300
H19	2.0346633381	2.8093705251	0.0916725528
H20	-0.1591856050	-2.7681752273	0.1147689825
H21	-2.5956243896	-2.7087368286	0.1372606105
H22	-3.8086535442	-0.5364848770	0.1473391610
H23	-2.5305541523	1.5798351312	0.1344083870

#####mol\_reduced#####

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structure

N1	3.7061900741	-1.8013103713	0.0786980448
C2	2.3537881388	-1.7497796779	0.0911200179
C3	1.5657215063	-0.5986795297	0.0977787931
C4	2.2461174532	0.6773970422	0.0908606463
C5	3.6775367489	0.6163089574	0.0777343479
C6	4.3208355358	-0.5991547532	0.0724381849
C7	0.0895817647	-0.6139759115	0.1113844031
C8	-0.6116694678	0.6511708600	0.1171757124
C9	0.1099446625	1.8600206264	0.1099041024
C10	1.5154351339	1.8693692293	0.0969646657
C11	-0.6645665219	-1.7928808106	0.1189648134
C12	-2.0641001720	-1.7941563170	0.1318734523
C13	-2.7443848911	-0.5682208410	0.1374788065
C14	-2.0405913439	0.6194793636	0.1303530571
H15	1.8721537555	-2.7246025711	0.0960595643
H16	4.2514341773	1.5395472140	0.0719900537
H17	5.4118237373	-0.6299286803	0.0624363737
H18	-0.4421222581	2.7962211499	0.1144982594
H19	2.0537585800	2.8140256483	0.0915223581
H20	-0.1520826735	-2.7485484418	0.1147539272
H21	-2.6102556698	-2.7318924516	0.1374231518
H22	-3.8319139872	-0.5507805106	0.1474916902
H23	-2.5728547736	1.5675887621	0.1347476589

#####mol\_double\_reduced#####

23

structure

N1	3.7477962088	-1.8268791557	0.0784539023
C2	2.3631794712	-1.7385143199	0.0911293503
C3	1.5804178458	-0.6009582723	0.0976579470
C4	2.2609497100	0.7067339417	0.0906694684
C5	3.7161106148	0.6076302038	0.0773390190
C6	4.3440122740	-0.6171435717	0.0722645206
C7	0.0762814717	-0.6137923300	0.1114753038
C8	-0.6278469458	0.6840807681	0.1173175580
C9	0.0854177316	1.8671912624	0.1101108474
C10	1.5381996819	1.8740874105	0.0966899121
C11	-0.6739212258	-1.7787892380	0.1189353760
C12	-2.1005806188	-1.8141618487	0.1321325370
C13	-2.7719542662	-0.5837287465	0.1377657466
C14	-2.0829166532	0.6154231620	0.1308153767
H15	1.8718246983	-2.7120930165	0.0962152189
H16	4.3113065062	1.5227944392	0.0713435574
H17	5.4439706373	-0.6378416426	0.0621584371
H18	-0.4578873765	2.8142234378	0.1146417353
H19	2.0704761262	2.8282593032	0.0912662332
H20	-0.1487410403	-2.7322824641	0.1145316099
H21	-2.6370003335	-2.7603682687	0.1375433651
H22	-3.8663732033	-0.5639685309	0.1478977709
H23	-2.6344456398	1.5571495414	0.1354791299

#####mol51#####

#####mol#####

23

structure

C1	3.6981333553	-1.7006684668	0.0759291748
C2	2.3224164372	-1.8037632882	0.0875267812
C3	1.5302023598	-0.6373718520	0.0970852529
C4	2.2263702113	0.5993279177	0.0940140498
C5	3.6390710736	0.5715042331	0.0817739797
N6	4.3680087656	-0.5280555646	0.0729071233
C7	0.0770649432	-0.6323618959	0.1095863225
C8	-0.6042730271	0.6182244207	0.1184090747
C9	0.1463491221	1.8411152494	0.1148737781
C10	1.5028180342	1.8341806284	0.1031764872
C11	-0.6935581212	-1.8147346133	0.1133815464
C12	-2.0729059618	-1.7706932874	0.1253172333
C13	-2.7418843525	-0.5351339441	0.1339954010
C14	-2.0161011329	0.6363014443	0.1305573265
H15	4.3127401256	-2.5958292873	0.0685381030
H16	1.8720294638	-2.7878272257	0.0890860306
H17	4.1813228470	1.5154662983	0.0793148103
H18	-0.3993447451	2.7786627096	0.1218090601
H19	2.0617722109	2.7639067062	0.1005771125
H20	-0.2008654852	-2.7786280899	0.1068514841



H21	-2.6414906828	-2.6935325755	0.1279967267
H22	-3.8253853329	-0.5052651460	0.1433540378
H23	-2.5243524776	1.5947927430	0.1371882907

#####mol\_reduced#####

23

structure

C1	3.7133843480	-1.6945603890	0.0758499829
C2	2.3401940329	-1.8156226996	0.0873301761
C3	1.5084077973	-0.6383134006	0.0972298759
C4	2.2471369926	0.6018412030	0.0938158244
C5	3.6386845612	0.5777354882	0.0818254485
N6	4.4130865815	-0.5385097172	0.0725561865
C7	0.0956945130	-0.6316719545	0.1093839364
C8	-0.6254882957	0.6276710460	0.1185967717
C9	0.1421253677	1.8436604879	0.1148903811
C10	1.4995544974	1.8351983633	0.1031731704
C11	-0.7108122745	-1.8262141251	0.1134681429
C12	-2.0860784771	-1.7688163441	0.1254392163
C13	-2.7753550015	-0.5360082380	0.1343232621
C14	-2.0223775454	0.6434687272	0.1306631344
H15	4.3191769880	-2.6027527774	0.0685367006
H16	1.9016609466	-2.8068574868	0.0887602231
H17	4.1751510365	1.5275469578	0.0794657425
H18	-0.3979584866	2.7884089886	0.1217914069
H19	2.0537615414	2.7713322006	0.1006270237
H20	-0.2230006415	-2.7941703208	0.1069418538
H21	-2.6543898983	-2.6966529011	0.1281039014
H22	-3.8596344209	-0.5065560162	0.1437406640
H23	-2.5256101486	1.6085609228	0.1373030098

#####mol\_double\_reduced#####

23

structure

C1	3.7294571319	-1.7106091981	0.0756573631
C2	2.3387731210	-1.8035793543	0.0873574805
C3	1.5151592083	-0.6218848292	0.0972263796
C4	2.2605874254	0.6317899376	0.0937976599
C5	3.6770810817	0.5687605629	0.0814747759
N6	4.4414802016	-0.5695244410	0.0722393358
C7	0.0845389092	-0.6223485541	0.1095102425
C8	-0.6348583803	0.6567389420	0.1187466436
C9	0.1193392735	1.8469346508	0.1150902354
C10	1.5317253873	1.8436371818	0.1029328997
C11	-0.7084955853	-1.8164939261	0.1134791481
C12	-2.1176000519	-1.7862699153	0.1256743975
C13	-2.7972773437	-0.5656017554	0.1344251741
C14	-2.0622629340	0.6391837928	0.1309732774
H15	4.3182698190	-2.6370345594	0.0684245310
H16	1.8845596694	-2.7907630325	0.0889160276
H17	4.2321134290	1.5119558554	0.0789115017

H18	-0.4177353744	2.7981586914	0.1219719475
H19	2.0801387730	2.7873543685	0.1004551168
H20	-0.2079982949	-2.7807440294	0.1068637203
H21	-2.6756858735	-2.7246645110	0.1282483133
H22	-3.8885313112	-0.5399698680	0.1438785953
H23	-2.5863385042	1.5967265273	0.1377601607

#####mol52#####

#####mol#####

23

structure

C1	3.6934310342	-1.7553760316	0.0768787760
C2	2.3177981586	-1.8385629781	0.0879431486
C3	1.5420457006	-0.6618835266	0.0977385285
C4	2.2548229101	0.5701886731	0.0954765668
N5	3.6083941674	0.6443861883	0.0845652649
C6	4.2926819144	-0.4842861754	0.0756506458
C7	0.0884067387	-0.6477139961	0.1097343745
C8	-0.5859706209	0.6060136030	0.1189606919
C9	0.1760711202	1.8211143945	0.1162383600
C10	1.5322401408	1.8074664958	0.1050384438
C11	-0.6925915572	-1.8240703383	0.1127123314
C12	-2.0718038022	-1.7696860753	0.1242362398
C13	-2.7331500878	-0.5300777659	0.1333333020
C14	-1.9975088522	0.6352406457	0.1306882246
H15	4.3077520579	-2.6478567057	0.0692303016
H16	1.8421849074	-2.8113468113	0.0890265321
H17	5.3759742662	-0.3914702666	0.0670194390
H18	-0.3622014059	2.7633568127	0.1234261388
H19	2.1169269423	2.7190857924	0.1028938893
H20	-0.2101688561	-2.7933435189	0.1058919883
H21	-2.6464456220	-2.6889606075	0.1262755321
H22	-3.8163997525	-0.4928395163	0.1423842347
H23	-2.4971397743	1.5983622841	0.1376408877

#####mol\_reduced#####

23

structure

C1	3.7256341507	-1.7648265269	0.0765790636
C2	2.3130652163	-1.8395447863	0.0879741479
C3	1.5506633147	-0.6696676406	0.0976498177
C4	2.2665749138	0.5867693842	0.0954287684
N5	3.6444679554	0.6484057901	0.0842757000
C6	4.3121626742	-0.5098428804	0.0754113716
C7	0.0831607003	-0.6392611906	0.1098083267
C8	-0.5993553478	0.6383547353	0.1191665252
C9	0.1464114230	1.8267499323	0.1165070074
C10	1.5447267273	1.7964748634	0.1049053611
C11	-0.6979874540	-1.8067113260	0.1128161941
C12	-2.0875127511	-1.7838022171	0.1243359056
C13	-2.7520508810	-0.5371062857	0.1334631274

C14	-2.0288378451	0.6308561897	0.1309211679
H15	4.3357092908	-2.6623938689	0.0689452933
H16	1.8333179491	-2.8115565127	0.0890913809
H17	5.4007838458	-0.4229576325	0.0667169868
H18	-0.3803577172	2.7775825768	0.1236303073
H19	2.1285227413	2.7109220696	0.1027774836
H20	-0.2004850368	-2.7708897612	0.1058777347
H21	-2.6528167935	-2.7098493712	0.1262786506
H22	-3.8387215445	-0.5021937164	0.1425205487
H23	-2.5425862374	1.5895770239	0.1379594750

#####mol\_double\_reduced#####

23

structure

C1	3.7261542790	-1.7664115464	0.0765855452
C2	2.3195688245	-1.8542043786	0.0879193364
C3	1.5334684646	-0.6503874710	0.0978595134
C4	2.2871095925	0.6032995483	0.0952995888
N5	3.6634205161	0.6644903995	0.0841324481
C6	4.3350111075	-0.5170612358	0.0751777644
C7	0.0991951860	-0.6335421424	0.1096989717
C8	-0.6124188688	0.6388489841	0.1192926034
C9	0.1511642218	1.8263339020	0.1164814399
C10	1.5594851239	1.8061590957	0.1048098047
C11	-0.7038137471	-1.8301319489	0.1127786481
C12	-2.1118417330	-1.7832893581	0.1245126949
C13	-2.7855879805	-0.5640123460	0.1336521968
C14	-2.0395886528	0.6400990145	0.1310555455
H15	4.3401012841	-2.6700633900	0.0689172158
H16	1.8378956769	-2.8262682513	0.0890915511
H17	5.4286625382	-0.4415341866	0.0663803081
H18	-0.3768314807	2.7821931157	0.1236332092
H19	2.1356379231	2.7304608535	0.1027597277
H20	-0.2144634805	-2.7988308593	0.1058749965
H21	-2.6775429042	-2.7180116547	0.1264152765
H22	-3.8767425118	-0.5340639428	0.1427241470
H23	-2.5534426494	1.6025923305	0.1381240131

#####mol53#####

#####mol#####

23

structure

C1	3.7062491766	-1.7498446200	0.0906680047
C2	2.3281532317	-1.8265413368	0.0981550443
C3	1.5333701517	-0.6602652748	0.1018094179
C4	2.1892941041	0.6020785589	0.0975816687
C5	3.5982350065	0.6566960281	0.0899327089
C6	4.3483768205	-0.4991291107	0.0865096746
C7	0.0832888625	-0.6702534938	0.1096215809
C8	-0.5796997204	0.5830589712	0.1125312148
C9	0.2171329370	1.7778329615	0.1076083613

N10	1.5131274096	1.8070694231	0.1005889101
C11	-0.7067929075	-1.8401364006	0.1144748585
C12	-2.0851041078	-1.7627816478	0.1218523625
C13	-2.7361354691	-0.5157733370	0.1247193208
C14	-1.9882961330	0.6415088580	0.1200921285
H15	4.2955708912	-2.6597838265	0.0879785885
H16	1.8557277179	-2.8010914282	0.1012418859
H17	4.0578024278	1.6376092740	0.0869100452
H18	5.4311021072	-0.4463976897	0.0806216661
H19	-0.2986462251	2.7380683769	0.1098918690
H20	-0.2338794047	-2.8139526095	0.1124255947
H21	-2.6725473409	-2.6741316999	0.1254783702
H22	-3.8188586597	-0.4700058656	0.1305247364
H23	-2.4726441625	1.6125706285	0.1222028496

#####mol\_reduced#####

23

structure

C1	3.7260280413	-1.7681951929	0.0905713684
C2	2.3305870263	-1.8114163048	0.0980932205
C3	1.5414302758	-0.6538226624	0.1017264588
C4	2.1963288994	0.6334888336	0.0975133535
C5	3.6239522015	0.6452038359	0.0898416884
C6	4.3653860448	-0.5196997723	0.0864781965
C7	0.0710624345	-0.6716396733	0.1096624249
C8	-0.5858887201	0.6134731435	0.1125366112
C9	0.1950617023	1.7775138774	0.1076933459
N10	1.5472373671	1.8193760219	0.1003652078
C11	-0.7073805018	-1.8288774332	0.1144694371
C12	-2.1130733434	-1.7845027674	0.1220480586
C13	-2.7533202228	-0.5358131962	0.1248677784
C14	-2.0192929649	0.6338923034	0.1202820992
H15	4.3028233724	-2.6877178239	0.0879553261
H16	1.8442972169	-2.7821235944	0.1012226897
H17	4.0999258460	1.6203805454	0.0867667354
H18	5.4519364779	-0.4670547762	0.0806126580
H19	-0.3118030879	2.7431278401	0.1099111971
H20	-0.2216876871	-2.7996024958	0.1123400903
H21	-2.6903224132	-2.7033802096	0.1256412663
H22	-3.8403575303	-0.4878952655	0.1307269864
H23	-2.5222927260	1.5976629511	0.1224957263

#####mol\_double\_reduced#####

23

structure

C1	3.7597479135	-1.7883826385	0.0904546918
C2	2.3374294303	-1.8002090149	0.0981383310
C3	1.5514412920	-0.6542029279	0.1016977389
C4	2.2087316234	0.6640967776	0.0974173767
C5	3.6632887706	0.6381186182	0.0895446876
C6	4.3925865129	-0.5390446692	0.0862917074

C7	0.0574553644	-0.6713906192	0.1097338609
C8	-0.5990881879	0.6470807761	0.1126244205
C9	0.1715784014	1.7845724707	0.1078791122
N10	1.5761444380	1.8258837109	0.1002306893
C11	-0.7160108824	-1.8168838199	0.1144535385
C12	-2.1481176882	-1.8092312364	0.1221864928
C13	-2.7787655752	-0.5538730606	0.1249841247
C14	-2.0620356771	0.6278039145	0.1205331648
H15	4.3265143239	-2.7172623341	0.0879423509
H16	1.8398099343	-2.7697410231	0.1014028815
H17	4.1577224089	1.6081620657	0.0862971152
H18	5.4856987987	-0.4857482333	0.0803403558
H19	-0.3182329843	2.7627307824	0.1100396080
H20	-0.2151616363	-2.7851234054	0.1122037736
H21	-2.7161857830	-2.7366162941	0.1257094849
H22	-3.8729865512	-0.5038211843	0.1308655864
H23	-2.5876701800	1.5840945488	0.1228925516

#####mol54#####

#####mol#####

22

structure

C1	3.5210032215	-1.7709655057	0.0853358512
N2	2.2011574728	-1.7819200914	0.0958191525
C3	1.5521695186	-0.5988635144	0.0976313442
C4	2.2395925477	0.6466289870	0.0886717563
C5	3.6491130250	0.6150757091	0.0776144438
C6	4.2989889179	-0.5976426857	0.0758854110
C7	0.0946860452	-0.5966461918	0.1091892838
C8	-0.5889903706	0.6509321330	0.1110433736
C9	0.1485482846	1.8792747733	0.1017154103
C10	1.5057440039	1.8772094824	0.0909907856
N11	-0.5578486396	-1.7777213867	0.1177448443
C12	-1.8776521866	-1.7627556076	0.1281724229
C13	-2.6521135469	-0.5870714403	0.1309340820
C14	-1.9985969701	0.6236613512	0.1222769766
H15	4.0077895850	-2.7434898402	0.0842087379
H16	4.2034304291	1.5480493238	0.0705961642
H17	5.3806999079	-0.6598574167	0.0675023307
H18	-0.4020051390	2.8143304105	0.1034093541
H19	2.0591016161	2.8105862006	0.0839723058
H20	-2.3673445413	-2.7337986719	0.1348499220
H21	-3.7340060421	-0.6459826496	0.1396848454
H22	-2.5501187775	1.5583134793	0.1239670330

#####mol\_reduced#####

22

structure

C1	3.5431870470	-1.7585495686	0.0851341936
N2	2.2228074738	-1.8103771563	0.0957507549
C3	1.5329894198	-0.6057647487	0.0978136515

C4	2.2536251305	0.6494350022	0.0885515118
C5	3.6453288032	0.6344359289	0.0775845216
C6	4.3272049568	-0.5959437508	0.0756495187
C7	0.1138443890	-0.6036116692	0.1090616338
C8	-0.6030137061	0.6537694121	0.1111462985
C9	0.1491444748	1.8786079693	0.1017039457
C10	1.5051608697	1.8765520864	0.0909886335
N11	-0.5795779126	-1.8061249125	0.1179903809
C12	-1.8998057836	-1.7502675397	0.1282964283
C13	-2.6803293488	-0.5852915266	0.1311496418
C14	-1.9947615370	0.6430107634	0.1222029652
H15	4.0468266641	-2.7295689727	0.0838708472
H16	4.1873143555	1.5775403611	0.0706367945
H17	5.4102662209	-0.6543722644	0.0672303902
H18	-0.4008142603	2.8177787017	0.1033813398
H19	2.0579269923	2.8140472043	0.0839609384
H20	-2.4063560928	-2.7197478592	0.1350873940
H21	-3.7635614056	-0.6404142476	0.1399039259
H22	-2.5339330436	1.5877519890	0.1237795978

#####mol\_double\_reduced#####

22

structure

C1	3.5663086804	-1.7699424736	0.0849846485
N2	2.2200066151	-1.8039893977	0.0957575333
C3	1.5432435584	-0.5980943852	0.0977117026
C4	2.2633793487	0.6743054282	0.0883927590
C5	3.6882286281	0.6337390270	0.0772211930
C6	4.3466712755	-0.6195286637	0.0755508339
C7	0.1036187479	-0.5958925234	0.1091317335
C8	-0.6127017069	0.6786937192	0.1111748003
C9	0.1241822783	1.8789803408	0.1019253506
C10	1.5300980235	1.8768315677	0.0907873102
N11	-0.5767552751	-1.7997215188	0.1179628812
C12	-1.9229499219	-1.7615939118	0.1285063455
C13	-2.6998556262	-0.6088094381	0.1313540954
C14	-2.0376609373	0.6424526185	0.1225474499
H15	4.0608509929	-2.7505527723	0.0838347723
H16	4.2471576021	1.5700648235	0.0701418262
H17	5.4361351659	-0.6912387683	0.0671218072
H18	-0.4214299008	2.8253299645	0.1035513861
H19	2.0785480449	2.8215129446	0.0837546479
H20	-2.4204187764	-2.7406981149	0.1352412649
H21	-3.7895303312	-0.6771902287	0.1401625866
H22	-2.5937987171	1.5804666364	0.1242679988

#####mol55#####

#####mol#####

22

structure

N1	3.5955824604	-1.8139395906	0.0823090985
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C2	2.2736525738	-1.7726957563	0.0927493184
C3	1.5194657804	-0.5789596267	0.0964672321
C4	2.2224825980	0.6505305182	0.0885177171
C5	3.6309760271	0.5942246151	0.0774298266
C6	4.2554722012	-0.6345218512	0.0748097144
C7	0.0713573342	-0.5766411578	0.1079765746
C8	-0.6141388139	0.6686197072	0.1109718375
C9	0.1346878837	1.8914655236	0.1026623544
C10	1.4927906326	1.8856193737	0.0919148155
N11	-0.5790414680	-1.7605852290	0.1154680485
C12	-1.9004949147	-1.7496577837	0.1259170457
C13	-2.6739273943	-0.5748297892	0.1297113339
C14	-2.0222399513	0.6385911115	0.1221613595
H15	1.7447651254	-2.7192225675	0.0987621444
H16	4.2138109177	1.5088003399	0.0710329877
H17	5.3394936225	-0.7009019940	0.0663140890
H18	-0.4106313268	2.8298019123	0.1051500567
H19	2.0477038441	2.8175291336	0.0857054736
H20	-2.3878724230	-2.7212527483	0.1317015362
H21	-3.7554194975	-0.6355520247	0.1383808437
H22	-2.5772910894	1.5711204729	0.1247094634

#####mol\_reduced#####

22

structure

N1	3.6123869489	-1.8358351578	0.0822406197
C2	2.2770445327	-1.7536672466	0.0926873417
C3	1.5264714496	-0.5718036757	0.0963801039
C4	2.2341064855	0.6857192313	0.0883373726
C5	3.6602364710	0.5865916581	0.0772152678
C6	4.2677308842	-0.6421732889	0.0747512930
C7	0.0619951923	-0.5839228590	0.1080477384
C8	-0.6238854586	0.6871649269	0.1110073754
C9	0.1207986157	1.8876235280	0.1027745143
C10	1.5228712339	1.8900855467	0.0916540540
N11	-0.5790235246	-1.7581932116	0.1154436392
C12	-1.9332677537	-1.7594166323	0.1261904828
C13	-2.6927061441	-0.5969510131	0.1299257101
C14	-2.0488972842	0.6375745725	0.1223951594
H15	1.7299097486	-2.6917868281	0.0988328944
H16	4.2609174539	1.4930233980	0.0706999853
H17	5.3557016209	-0.7082056447	0.0662442997
H18	-0.4222097620	2.8298797521	0.1052461242
H19	2.0681587180	2.8301996641	0.0855100777
H20	-2.4096203917	-2.7373939417	0.1318880371
H21	-3.7781686973	-0.6581371575	0.1386472864
H22	-2.6144759773	1.5651107966	0.1250583032

#####mol\_double\_reduced#####

22

structure

N1	3.6543242607	-1.8610034703	0.0819500125
C2	2.2867412960	-1.7396894347	0.0925909055
C3	1.5423375935	-0.5749332525	0.0962786967
C4	2.2505290748	0.7157723969	0.0881544613
C5	3.6988837968	0.5777991209	0.0769039872
C6	4.2908785499	-0.6598796943	0.0745812319
C7	0.0459171442	-0.5867280794	0.1082000069
C8	-0.6404998993	0.7177691638	0.1110972763
C9	0.0963418525	1.8931504501	0.1029774031
C10	1.5465014413	1.8934915753	0.0914614831
N11	-0.5895577778	-1.7458575043	0.1155111618
C12	-1.9696561089	-1.7776954182	0.1265083518
C13	-2.7183858643	-0.6091723147	0.1301341814
C14	-2.0916106622	0.6341345894	0.1227305475
H15	1.7294628432	-2.6749152375	0.0988117783
H16	4.3202866445	1.4758241865	0.0702257049
H17	5.3879908319	-0.7158031370	0.0659734135
H18	-0.4376805255	2.8463300298	0.1053571843
H19	2.0848267610	2.8439164766	0.0853320886
H20	-2.4331336747	-2.7640711513	0.1321069037
H21	-3.8113836123	-0.6699095151	0.1388917541
H22	-2.6754578041	1.5548888626	0.1255258549

#####mol56#####

#####mol#####

22

structure

C1	3.6210220741	-1.7420606935	0.0781172460
C2	2.2431894612	-1.8128254804	0.0880097172
C3	1.4986749440	-0.6202044172	0.0950833013
C4	2.2113649849	0.6032276328	0.0916350083
C5	3.6236302853	0.5390672315	0.0812941171
N6	4.3179120053	-0.5828136185	0.0746829206
C7	0.0491137344	-0.5935954936	0.1056231375
C8	-0.6167565574	0.6617527448	0.1121973184
C9	0.1454654038	1.8769825357	0.1083912220
C10	1.5034572634	1.8486558724	0.0985156131
N11	-0.6147289621	-1.7695988207	0.1087751326
C12	-1.9357033807	-1.7434900877	0.1183521320
C13	-2.6923580454	-0.5573308562	0.1254797483
C14	-2.0260733456	0.6476872620	0.1223597902
H15	4.2175992637	-2.6491747453	0.0725172603
H16	1.7254169762	-2.7626219662	0.0904275661
H17	4.1939496473	1.4664132673	0.0784418626
H18	-0.3878948446	2.8218007369	0.1135808097
H19	2.0743598564	2.7711531716	0.0956748843
H20	-2.4363048138	-2.7082676822	0.1206152798
H21	-3.7747213507	-0.6035819697	0.1332309168
H22	-2.5699766477	1.5866596544	0.1276108949

#####mol\_reduced#####



22

structure

C1	3.6234202846	-1.7390765649	0.0780773137
C2	2.2558763007	-1.8076360097	0.0879131716
C3	1.4778802198	-0.6122582028	0.0952592645
C4	2.2281542282	0.6201074470	0.0915488777
C5	3.6339314228	0.5428884565	0.0812428973
N6	4.3504974856	-0.5721130026	0.0744582626
C7	0.0530657145	-0.6045299589	0.1056015402
C8	-0.6309886652	0.6618820091	0.1123032647
C9	0.1540583013	1.8706910835	0.1083123677
C10	1.5230013040	1.8512266231	0.0983775294
N11	-0.6241659615	-1.7989149194	0.1088340379
C12	-1.9696104788	-1.7406472169	0.1186236803
C13	-2.7175841000	-0.5787092055	0.1256289219
C14	-2.0307792339	0.6622900797	0.1224002227
H15	4.2172634775	-2.6512292486	0.0724601224
H16	1.7373896110	-2.7585503816	0.0903201578
H17	4.1985655780	1.4785367393	0.0784681104
H18	-0.3784046665	2.8192602620	0.1134810774
H19	2.0869526890	2.7814057537	0.0955951529
H20	-2.4766722509	-2.7069640922	0.1209371257
H21	-3.8022904840	-0.6237991520	0.1333857918
H22	-2.5711054739	1.6047313293	0.1275969560

#####mol\_double\_reduced#####

22

structure

C1	3.6546181261	-1.7453112807	0.0778896347
C2	2.2632123114	-1.8088330278	0.0878542501
C3	1.4814944772	-0.6057474800	0.0951998458
C4	2.2416697357	0.6321093471	0.0914583798
C5	3.6567922352	0.5377148755	0.0810916425
N6	4.3905083282	-0.6200517491	0.0741556689
C7	0.0541997334	-0.5913767634	0.1055386698
C8	-0.6456447499	0.6958643958	0.1124301392
C9	0.1189185401	1.8756553584	0.1085609624
C10	1.5298158107	1.8569614881	0.0983331994
N11	-0.6290116120	-1.7926641305	0.1087895608
C12	-1.9786954062	-1.7488153279	0.1186706649
C13	-2.7390453414	-0.5818145868	0.1258294180
C14	-2.0722317518	0.6644877582	0.1227272299
H15	4.2260955334	-2.6826547097	0.0724379052
H16	1.7432930741	-2.7601778331	0.0902663927
H17	4.2355039749	1.4664917287	0.0782105897
H18	-0.4088910776	2.8325982918	0.1137260606
H19	2.0905600974	2.7931842010	0.0956046294
H20	-2.4845897239	-2.7219836672	0.1209903451
H21	-3.8291334646	-0.6401165672	0.1336689821
H22	-2.6271468215	1.6033782341	0.1280606739

#####mol57#####

#####mol#####

22

structure

C1	3.6164966901	-1.7925274429	0.0785193898
C2	2.2399071732	-1.8462639943	0.0880180371
C3	1.5110089225	-0.6428403474	0.0954930196
C4	2.2398001002	0.5745670423	0.0928240978
N5	3.5953518828	0.6167924807	0.0834595653
C6	4.2454225040	-0.5330787231	0.0766371342
C7	0.0626238617	-0.6078559397	0.1056722963
C8	-0.5974735101	0.6504098181	0.1127186097
C9	0.1756449901	1.8584707615	0.1097185555
C10	1.5331387946	1.8235999511	0.1002142395
N11	-0.6097256070	-1.7804629416	0.1080893373
C12	-1.9306146267	-1.7451861623	0.1173574324
C13	-2.6807741190	-0.5553746926	0.1248673052
C14	-2.0065187039	0.6455515173	0.1224984485
H15	4.2144561070	-2.6960167210	0.0725501284
H16	1.6969731723	-2.7826216821	0.0899485788
H17	5.3308665060	-0.4694918626	0.0691936877
H18	-0.3508637674	2.8073241894	0.1152448685
H19	2.1305256452	2.7270281062	0.0978459369
H20	-2.4373490666	-2.7067885791	0.1190374663
H21	-3.7632695608	-0.5959588156	0.1323175929
H22	-2.5440389628	1.5882270632	0.1280623361

#####mol\_reduced#####

22

structure

C1	3.6320771100	-1.8041668686	0.0783982234
C2	2.2366406989	-1.8277447302	0.0880845369
C3	1.5165404076	-0.6363557735	0.0954646123
C4	2.2568817659	0.6070711113	0.0927618488
N5	3.6393162188	0.6154538708	0.0831516764
C6	4.2615380443	-0.5475664181	0.0765088388
C7	0.0501618592	-0.6129550642	0.1057398004
C8	-0.6092106077	0.6706832975	0.1128421199
C9	0.1605218417	1.8501289564	0.1098052098
C10	1.5627356001	1.8223320287	0.0999933306
N11	-0.6098518972	-1.7767241478	0.1080756160
C12	-1.9631355390	-1.7568276973	0.1175523655
C13	-2.7013744650	-0.5765389769	0.1249827841
C14	-2.0393974425	0.6441049387	0.1227403097
H15	4.2186314551	-2.7166906601	0.0724870690
H16	1.6784871370	-2.7572578701	0.0901341801
H17	5.3533532520	-0.4986091260	0.0690048619
H18	-0.3596571458	2.8053437825	0.1153058174
H19	2.1454679250	2.7372419410	0.0977481986
H20	-2.4589255349	-2.7253145989	0.1191360100

H21	-3.7880599703	-0.6196499706	0.1324716011
H22	-2.5890677257	1.5812239263	0.1283876996

#####mol\_double\_reduced#####

22

structure

C1	3.6535825272	-1.7968491531	0.0782870365
C2	2.2458004559	-1.8545993927	0.0879856382
C3	1.5006463424	-0.6331335916	0.0955844976
C4	2.2695093162	0.6044680127	0.0926440251
N5	3.6461985108	0.6369002879	0.0830915533
C6	4.2892939777	-0.5617637128	0.0762669132
C7	0.0691666502	-0.6019384107	0.1056460159
C8	-0.6228011851	0.6783473093	0.1129855001
C9	0.1508079983	1.8556363700	0.1099036514
C10	1.5578355857	1.8204925538	0.1000112256
N11	-0.6219879434	-1.8067701693	0.1081022460
C12	-1.9705475032	-1.7490173243	0.1175945230
C13	-2.7252595610	-0.5825793050	0.1251308634
C14	-2.0492169805	0.6641172984	0.1228818683
H15	4.2496419882	-2.7125058234	0.0723455474
H16	1.6990646079	-2.7895043090	0.0899660237
H17	5.3843506505	-0.5101286809	0.0687343579
H18	-0.3674007174	2.8173407388	0.1154131194
H19	2.1447223835	2.7378381274	0.0977265154
H20	-2.4838359274	-2.7190685611	0.1192552429
H21	-3.8155583483	-0.6369816725	0.1325995627
H22	-2.5953671551	1.6076196814	0.1285315456

#####mol58#####

#####mol#####

22

structure

C1	3.6318273957	-1.7852874160	0.0930185552
C2	2.2527666850	-1.8326321423	0.0989557754
C3	1.5015954062	-0.6413403934	0.0996566390
C4	2.1743491698	0.6097632624	0.0942070566
C5	3.5841113376	0.6314216302	0.0882042755
C6	4.3010793100	-0.5466526869	0.0876184884
C7	0.0573102742	-0.6295338393	0.1057175625
C8	-0.5922080952	0.6283761033	0.1058242809
C9	0.2160202204	1.8157774981	0.0999677115
N10	1.5130898334	1.8242187200	0.0944753287
N11	-0.6246226670	-1.7967952620	0.1110127426
C12	-1.9450474089	-1.7398466833	0.1164186576
C13	-2.6855228851	-0.5416214020	0.1170178177
C14	-1.9986554452	0.6521787442	0.1116618566
H15	4.2039406020	-2.7061520504	0.0925043043
H16	1.7185862594	-2.7741003441	0.1031692069
H17	4.0718431494	1.5986022951	0.0841366274
H18	5.3850072667	-0.5202802352	0.0829761456

H19	-0.2870967695	2.7828200564	0.1000924950
H20	-2.4650592958	-2.6947365440	0.1205833730
H21	-3.7681733898	-0.5736860849	0.1216136183
H22	-2.5214208451	1.6033855046	0.1118745537

#####mol\_reduced#####

22

structure

C1	3.6397412065	-1.8000429793	0.0930291753
C2	2.2542130046	-1.8141627557	0.0989262317
C3	1.5050482192	-0.6265919654	0.0996157880
C4	2.1826121236	0.6421436071	0.0941036856
C5	3.6091287996	0.6217046145	0.0880984309
C6	4.3149270765	-0.5600762650	0.0875774908
C7	0.0442179722	-0.6369025282	0.1057902994
C8	-0.5982049574	0.6500659591	0.1058159798
C9	0.2043302396	1.8061935805	0.1000463087
N10	1.5508975951	1.8381839131	0.0942909890
N11	-0.6155381270	-1.7964599079	0.1109648668
C12	-1.9773158234	-1.7544801818	0.1165670333
C13	-2.7010246723	-0.5679454298	0.1171307803
C14	-2.0298256970	0.6517844224	0.1118065772
H15	4.2000283953	-2.7299245034	0.0925920962
H16	1.6998504721	-2.7462909590	0.1032145334
H17	4.1113551810	1.5839854905	0.0839582280
H18	5.4023263583	-0.5380288237	0.0829149112
H19	-0.2935357690	2.7772421529	0.1001367076
H20	-2.4850969265	-2.7164431061	0.1206729222
H21	-3.7881585085	-0.6024735305	0.1217363883
H22	-2.5679765387	1.5952098262	0.1121040489

#####mol\_double\_reduced#####

22

structure

C1	3.6708063721	-1.8199462826	0.0929252897
C2	2.2606830118	-1.7993217750	0.0988252388
C3	1.5158223121	-0.6257676891	0.0995368761
C4	2.1967392151	0.6745036191	0.0939868132
C5	3.6483573062	0.6136041084	0.0880144506
C6	4.3413637236	-0.5789896402	0.0875441649
C7	0.0269464945	-0.6402060374	0.1058286224
C8	-0.6121317084	0.6810343959	0.1057818418
C9	0.1813763457	1.8119322228	0.1001000920
N10	1.5832591149	1.8455021819	0.0941383141
N11	-0.6243269516	-1.7862441216	0.1109575865
C12	-2.0125235216	-1.7785105938	0.1168070471
C13	-2.7240376541	-0.5846333350	0.1173107308
C14	-2.0715945610	0.6450892331	0.1119924850
H15	4.2206129007	-2.7590288650	0.0925456855
H16	1.6928600431	-2.7275484896	0.1031389077
H17	4.1692101658	1.5702228442	0.0838563533

H18	5.4351170998	-0.5572924889	0.0828899057
H19	-0.2999068263	2.7947760879	0.1000808789
H20	-2.5054015860	-2.7501522343	0.1209208804
H21	-3.8190285254	-0.6176393249	0.1219935740
H22	-2.6321422212	1.5799348564	0.1123892603

#####mol59#####

#####mol#####

22

structure

C1	3.6485409244	-1.8005797208	0.0927239007
C2	2.2688617042	-1.8459022257	0.0987001993
C3	1.5254850317	-0.6501247064	0.0998853854
C4	2.2053660470	0.5914685152	0.0949511831
C5	3.6155826999	0.6141521506	0.0888883478
C6	4.3281631253	-0.5665932537	0.0877782184
C7	0.0798602006	-0.6183509056	0.1059537010
C8	-0.5595363886	0.6483291179	0.1066166201
N9	0.1261283534	1.8461490316	0.1017692441
C10	1.4239948474	1.7975128896	0.0963175168
N11	-0.6077267476	-1.7809096558	0.1107334383
C12	-1.9287043346	-1.7217060776	0.1162096608
C13	-2.6584615311	-0.5187011132	0.1173597020
C14	-1.9666063861	0.6727311516	0.1125285656
H15	4.2174033654	-2.7236924052	0.0918118791
H16	1.7312379361	-2.7851244934	0.1025523867
H17	4.1289401567	1.5700700849	0.0851242401
H18	5.4119689798	-0.5486685323	0.0830992906
H19	1.9515663786	2.7510816551	0.0925239042
H20	-2.4520012078	-2.6745164985	0.1199408576
H21	-3.7417578948	-0.5420678099	0.1219729687
H22	-2.4633458124	1.6358444230	0.1130833164

#####mol\_reduced#####

22

structure

C1	3.6644892249	-1.8189219356	0.0927087399
C2	2.2723601528	-1.8310080246	0.0986541802
C3	1.5312891082	-0.6448678722	0.0998364645
C4	2.2134772302	0.6247389029	0.0948523132
C5	3.6452928416	0.6071990821	0.0887734366
C6	4.3431629480	-0.5772116669	0.0877565487
C7	0.0719101212	-0.6222916001	0.1059755109
C8	-0.5666527946	0.6722488905	0.1066049968
N9	0.1036856568	1.8510912439	0.1018515497
C10	1.4521406903	1.8007210128	0.0961834419
N11	-0.6073651168	-1.7780979812	0.1107013190
C12	-1.9555472877	-1.7342083642	0.1163372549
C13	-2.6747281042	-0.5434034712	0.1174925114
C14	-1.9892937777	0.6666051578	0.1126597691
H15	4.2240046071	-2.7488557606	0.0918662713

H16	1.7195085803	-2.7638531925	0.1025550877
H17	4.1758322197	1.5564452224	0.0849398463
H18	5.4307847836	-0.5603609904	0.0830822841
H19	1.9676668409	2.7616134144	0.0924232501
H20	-2.4672392278	-2.6947821435	0.1200226963
H21	-3.7619420148	-0.5673136038	0.1221414690
H22	-2.4996924783	1.6236812121	0.1133073776

#####mol\_double\_reduced#####

22

structure

C1	3.6988074308	-1.8417216020	0.0925377172
C2	2.2802629995	-1.8171721978	0.0985260044
C3	1.5438469523	-0.6450719622	0.0997756369
C4	2.2275198220	0.6582039691	0.0947624927
C5	3.6871856276	0.6011174265	0.0886470595
C6	4.3684791557	-0.5954484598	0.0876749097
C7	0.0604535577	-0.6256421647	0.1060580847
C8	-0.5789808716	0.7005960554	0.1065903019
N9	0.0755394994	1.8568354466	0.1019443258
C10	1.4759230210	1.8065385308	0.0960895037
N11	-0.6146433520	-1.7705422257	0.1108094756
C12	-1.9884363182	-1.7517926680	0.1165919921
C13	-2.6993480402	-0.5602387051	0.1176093172
C14	-2.0276007280	0.6613763456	0.1127470380
H15	4.2497123673	-2.7794622217	0.0916953273
H16	1.7117420385	-2.7450180966	0.1024333313
H17	4.2394002107	1.5426875326	0.0847760660
H18	5.4631460829	-0.5769069873	0.0829856296
H19	1.9746282128	2.7802712331	0.0923878414
H20	-2.4876791938	-2.7216066524	0.1203104292
H21	-3.7937155762	-0.5858815597	0.1222586891
H22	-2.5549123470	1.6131380729	0.1133794834

#####mol60#####

#####mol#####

22

structure

C1	3.6413262959	-1.7995129099	0.0886905163
C2	2.2612594649	-1.8281438202	0.0921630835
C3	1.5223155479	-0.6289787153	0.0990005489
C4	2.2088830172	0.6150135260	0.1023182678
C5	3.6204691948	0.6149255217	0.0986438344
C6	4.3259787723	-0.5706608311	0.0919437474
C7	0.0736132495	-0.6252607529	0.1027731448
C8	-0.6292646220	0.6107274731	0.1096324073
C9	0.0994441694	1.8430540819	0.1127687820
C10	1.4576319360	1.8390084708	0.1092489375
N11	-0.5940827618	-1.7981360434	0.0997224992
C12	-1.9135011156	-1.7383056786	0.1033645285
C13	-2.6077169801	-0.5136543869	0.1101532555

N14	-1.9819731731	0.6490132286	0.1132913295
H15	4.2009693128	-2.7279972809	0.0834286306
H16	1.7181330733	-2.7642572063	0.0897395305
H17	4.1446407173	1.5648568801	0.1011699652
H18	5.4100433195	-0.5565117175	0.0891770141
H19	-0.4745770209	2.7616591418	0.1179929163
H20	2.0053567395	2.7757871447	0.1116515111
H21	-2.4547412303	-2.6806097077	0.1009133116
H22	-3.6942892604	-0.4950651053	0.1130264755

#####mol\_reduced#####

22

structure

C1	3.6404125829	-1.8059727730	0.0886614480
C2	2.2623908847	-1.8107655392	0.0922300428
C3	1.5145787819	-0.6106219407	0.0990980844
C4	2.2224474621	0.6446698565	0.1023938943
C5	3.6442357264	0.6131217321	0.0985733919
C6	4.3406631661	-0.5718521854	0.0919021853
C7	0.0673052734	-0.6345829975	0.1027587696
C8	-0.6409383402	0.6136572639	0.1096650115
C9	0.1007608800	1.8244104702	0.1127000902
C10	1.4848401545	1.8475629678	0.1092209324
N11	-0.5790634686	-1.8246360855	0.0996017346
C12	-1.9401516833	-1.7392152519	0.1034539809
C13	-2.6189673915	-0.5419310444	0.1100522662
N14	-2.0109774465	0.6696062707	0.1134072980
H15	4.1912355462	-2.7419482514	0.0833868563
H16	1.6999852919	-2.7371851127	0.0898955206
H17	4.1793611516	1.5602833159	0.1010703913
H18	5.4273387899	-0.5650703649	0.0891101901
H19	-0.4765145479	2.7441190282	0.1179533920
H20	2.0186599759	2.7946572937	0.1117217484
H21	-2.4846586057	-2.6826066815	0.1010373015
H22	-3.7096257169	-0.5345793727	0.1128829108

#####mol\_double\_reduced#####

22

structure

C1	3.6797671530	-1.8263442329	0.0884922738
C2	2.2748843331	-1.7914973851	0.0922867010
C3	1.5336170524	-0.6126740576	0.0990386553
C4	2.2420125921	0.6794554071	0.1024850105
C5	3.6899719375	0.6086080189	0.0984230467
C6	4.3706804253	-0.5848745292	0.0917647539
C7	0.0487151969	-0.6465678283	0.1027556966
C8	-0.6603439582	0.6386855383	0.1098232441
C9	0.0747212711	1.8191936846	0.1127526950
C10	1.5136226787	1.8507866256	0.1091645456
N11	-0.5833637805	-1.8096219117	0.0996590023
C12	-1.9829024117	-1.7560899521	0.1034787436

C13	-2.6443653259	-0.5557170539	0.1100629450
N14	-2.0652211261	0.6634467226	0.1135364176
H15	4.2210290584	-2.7703082730	0.0832254338
H16	1.6985422662	-2.7137271374	0.0900193111
H17	4.2456387449	1.5485764791	0.1008150344
H18	5.4640634173	-0.5745873456	0.0889498712
H19	-0.4944718872	2.7491370970	0.1180305942
H20	2.0346337617	2.8102495352	0.1117512661
H21	-2.5122096218	-2.7101121878	0.1009590724
H22	-3.7458030185	-0.5589056724	0.1128824979

#####mol61#####

#####mol#####

22

structure

C1	3.6382944036	-1.8027791742	0.0877909391
C2	2.2585131655	-1.8186447688	0.0905431615
C3	1.5315288023	-0.6123504625	0.0984372127
C4	2.2278229148	0.6270660346	0.1035703931
C5	3.6395086656	0.6131421747	0.1006037234
C6	4.3329108450	-0.5792960063	0.0928571507
C7	0.0839784719	-0.5966973637	0.1015199981
C8	-0.6003853025	0.6435410297	0.1094955159
C9	0.1322036063	1.8728364743	0.1144864986
C10	1.4903174191	1.8598806245	0.1116169696
N11	-0.5975201154	-1.7638850645	0.0967743474
C12	-1.9149256339	-1.6894686139	0.0999099977
N13	-2.6711457585	-0.5713762288	0.1073948777
C14	-2.0063885517	0.5704779225	0.1120431236
H15	4.1902713506	-2.7356481061	0.0817099114
H16	1.7043444926	-2.7482007791	0.0867525641
H17	4.1735942021	1.5574605944	0.1045230121
H18	5.4170844249	-0.5746695497	0.0906668674
H19	-0.4159008303	2.8091323482	0.1205813639
H20	2.0473209685	2.7908213423	0.1154064661
H21	-2.4573900591	-2.6303126962	0.0960714600
H22	-2.5960535665	1.4857595144	0.1181252992

#####mol\_reduced#####

22

structure

C1	3.6373584741	-1.8053125101	0.0877756976
C2	2.2653084873	-1.8107737434	0.0905719331
C3	1.5160292867	-0.5980692622	0.0985636753
C4	2.2453075017	0.6529580068	0.1036833065
C5	3.6595138682	0.6164051667	0.1005780783
C6	4.3546590991	-0.5738751690	0.0928371465
C7	0.0907252542	-0.5990905512	0.1015110553
C8	-0.6153491209	0.6462309494	0.1095592580
C9	0.1387993450	1.8676925312	0.1144445146
C10	1.5133077870	1.8660156411	0.1115963745



N11	-0.6012844687	-1.7865887088	0.0966568070
C12	-1.9387803986	-1.6878016714	0.0999525190
N13	-2.7032497206	-0.6070781766	0.1072580038
C14	-2.0147432166	0.5802582273	0.1121129540
H15	4.1848501250	-2.7439571827	0.0816590161
H16	1.7011003285	-2.7356639375	0.0868137585
H17	4.1985912647	1.5617601993	0.1044707784
H18	5.4405651842	-0.5765161306	0.0905855695
H19	-0.4066666066	2.8086757370	0.1205377125
H20	2.0604196136	2.8062511760	0.1154306514
H21	-2.4692222693	-2.6429787520	0.0959924226
H22	-2.6094793645	1.4913583132	0.1181690611

#####mol\_double\_reduced#####

22

structure

C1	3.6853659429	-1.8118138962	0.0876475747
C2	2.2776402525	-1.8160543399	0.0905674519
C3	1.5228007270	-0.6026747952	0.0985519356
C4	2.2559038766	0.6614136520	0.1037068068
C5	3.6815389119	0.6165032094	0.1004947862
C6	4.3894781723	-0.6063827316	0.0925497577
C7	0.0933527822	-0.5880882268	0.1015865760
C8	-0.6305804873	0.6724794935	0.1097387183
C9	0.1045566120	1.8741730079	0.1145863291
C10	1.5171148204	1.8655063922	0.1116141426
N11	-0.6172018767	-1.7837238981	0.0967319124
C12	-1.9496351054	-1.6905719732	0.0999350211
N13	-2.7349115760	-0.6080695355	0.1072584838
C14	-2.0445898401	0.5812521715	0.1121459763
H15	4.2272205368	-2.7600464115	0.0815008216
H16	1.7179217347	-2.7446545809	0.0868283781
H17	4.2269256331	1.5619618198	0.1043567555
H18	5.4811773578	-0.6036069225	0.0902808664
H19	-0.4370307994	2.8227020917	0.1207352770
H20	2.0653883754	2.8098052088	0.1154886915
H21	-2.4815944977	-2.6523046616	0.0959333381
H22	-2.6437566239	1.4958931934	0.1182161482

#####mol62#####

#####mol#####

22

structure

C1	3.6108935281	-1.8043478867	0.0885008513
C2	2.2299145554	-1.8086422591	0.0906537578
C3	1.5145134309	-0.5964209118	0.0982001991
C4	2.2257096203	0.6327283968	0.1036191190
C5	3.6365417923	0.6084640229	0.1012760869
C6	4.3196353609	-0.5902266093	0.0938281331
C7	0.0626355787	-0.5596046552	0.1006482799
C8	-0.6123985378	0.6901235537	0.1083314506

C9	0.1424558546	1.9078007255	0.1136457300
C10	1.4995890146	1.8729537570	0.1113572447
N11	-0.5985490932	-1.7374877869	0.0954001599
N12	-1.9096803531	-1.7714897489	0.0972158258
C13	-2.6041764434	-0.6147354117	0.1044218887
C14	-2.0103576981	0.6306732715	0.1101477228
H15	4.1519858308	-2.7436324610	0.0826644347
H16	1.6692924434	-2.7338527314	0.0866292146
H17	4.1780785841	1.5485875880	0.1054200357
H18	5.4036749828	-0.5967113765	0.0920838765
H19	-0.3903883966	2.8526144647	0.1194961403
H20	2.0675058562	2.7976061501	0.1154058531
H21	-3.6818879866	-0.7334243985	0.1054262784
H22	-2.6075821868	1.5362075332	0.1158738824

#####mol\_reduced#####

22

structure

C1	3.6205077126	-1.8131129030	0.0884368324
C2	2.2359451822	-1.7885551657	0.0907374034
C3	1.5175139618	-0.5805983605	0.0982850645
C4	2.2388774866	0.6645862828	0.1037894928
C5	3.6628055581	0.6049715115	0.1012388750
C6	4.3357434144	-0.5951609613	0.0937886157
C7	0.0514569670	-0.5707142243	0.1005950486
C8	-0.6143327338	0.7043995648	0.1083953378
C9	0.1362307907	1.8932697171	0.1135618044
C10	1.5312368707	1.8859464258	0.1113742670
N11	-0.5888771072	-1.7435211445	0.0953382696
N12	-1.9581738879	-1.7933664342	0.0971737162
C13	-2.6165537953	-0.6311696615	0.1043716081
C14	-2.0386876488	0.6275368451	0.1101753720
H15	4.1529303431	-2.7590846049	0.0825745274
H16	1.6546536770	-2.7030377861	0.0867903443
H17	4.2168734934	1.5407951179	0.1053412527
H18	5.4228691989	-0.6056058794	0.0920245026
H19	-0.3994716524	2.8404232136	0.1194138688
H20	2.0868497626	2.8194294932	0.1154789830
H21	-3.7025545211	-0.7333489947	0.1055058040
H22	-2.6472573936	1.5270596606	0.1158954648

#####mol\_double\_reduced#####

22

structure

C1	3.6566095420	-1.8305486100	0.0881707405
C2	2.2485581138	-1.7699947238	0.0907274909
C3	1.5314244194	-0.5804874239	0.0982601590
C4	2.2585395807	0.6995389256	0.1039334335
C5	3.7053035335	0.6012638411	0.1011685384
C6	4.3651948883	-0.6070054568	0.0936506920
C7	0.0342993766	-0.5801375941	0.1006652662

C8	-0.6291330971	0.7288135493	0.1085219082
C9	0.1162043473	1.8917073815	0.1135224866
C10	1.5605685495	1.8919178447	0.1113396995
N11	-0.5981910223	-1.7362781919	0.0956124722
N12	-2.0103982673	-1.8172587567	0.0972760494
C13	-2.6415535802	-0.6441546864	0.1043163956
C14	-2.0765273893	0.6206806419	0.1101013252
H15	4.1791564385	-2.7846120171	0.0821963737
H16	1.6554494298	-2.6810167736	0.0867662563
H17	4.2775210714	1.5311094328	0.1052732071
H18	5.4588417808	-0.6147779438	0.0919027972
H19	-0.4142231244	2.8479569147	0.1193717952
H20	2.1049124961	2.8376968949	0.1155532813
H21	-3.7382733283	-0.7324910114	0.1054493161
H22	-2.7019864378	1.5136430429	0.1157044136

#####mol63#####

#####mol#####

23

structure

C1	0.1759795668	0.1582233599	0.0092727240
C2	0.1712566949	1.4960697801	0.4273099154
C3	-0.9723505402	2.2711086648	0.2932510498
C4	-2.1224368300	1.7250215380	-0.2795595718
C5	-2.1224457318	0.4027646811	-0.7163083567
C6	-0.9805680038	-0.3806011239	-0.5678350037
C7	1.4525305783	-0.6155460182	0.1423784535
O8	2.5158865255	-0.0520222420	0.2941912962
C9	1.4132106277	-2.1323125859	0.1150022478
C10	0.5112349912	-2.8464089629	0.9089192357
C11	0.6012443106	-4.2350375186	0.9388121527
C12	1.5667623370	-4.8567203589	0.1561926315
H13	1.0806451824	1.9045156356	0.8508115431
H14	-0.9702114412	3.3021275832	0.6283810452
H15	-3.0139822021	2.3322312399	-0.3898181959
H16	-3.0096913462	-0.0180873924	-1.1753462600
H17	-0.9846121296	-1.4043882096	-0.9210049467
H18	-0.2297161208	-2.3239633769	1.5011033031
H19	-0.0702646538	-4.8170967321	1.5595567454
H20	1.6720051467	-5.9352305536	0.1403253173
N21	2.3527094581	-2.7246137222	-0.6334228010
C23	2.4095096723	-4.0559954373	-0.6158347226
H24	3.1711313428	-4.5073817108	-1.2457820488

#####mol\_reduced#####

23

structure

C1	0.1427872680	0.1121323209	-0.0075627813
C2	0.2048367050	1.4851112181	0.3395180503
C3	-0.9165060886	2.2989063027	0.3103344713
C4	-2.1595400637	1.7933434897	-0.0898851069

C5	-2.2374932641	0.4512519768	-0.4761483238
C6	-1.1161791147	-0.3696029284	-0.4397722700
C7	1.4191518281	-0.6487032934	0.0039878288
O8	2.5015688537	-0.0028344579	-0.0128214954
C9	1.4262993346	-2.1171527145	0.0495960921
C10	0.3665793353	-2.8945971764	0.5972234399
C11	0.4689615368	-4.2684833712	0.6739625782
C12	1.6358266302	-4.8981601496	0.2047097149
H13	1.1773020316	1.8714552804	0.6193852565
H14	-0.8269059464	3.3438913163	0.5978690966
H15	-3.0373148127	2.4313657513	-0.1182407792
H16	-3.1824551598	0.0438019579	-0.8271458151
H17	-1.2066755762	-1.3896394004	-0.7919960647
H18	-0.5056271328	-2.3993404673	1.0038953887
H19	-0.3369502130	-4.8498190054	1.1148495372
H20	1.7673212381	-5.9742134142	0.2396976117
N21	2.5778945517	-2.7412031128	-0.3627070409
C23	2.6438219754	-4.0628551574	-0.2826218590
H24	3.5786206121	-4.5070169293	-0.6332002632

#####mol\_double\_reduced#####

23

structure

C1	0.1367735985	0.0795087885	0.0168084167
C2	0.2197621928	1.5071790497	0.2157036831
C3	-0.8852734549	2.3351668977	0.1851830319
C4	-2.1801588293	1.8395869589	-0.0791337333
C5	-2.2837753613	0.4570171509	-0.3532507707
C6	-1.1823457119	-0.3837445848	-0.3159635980
C7	1.4089806408	-0.6533416225	0.0469042946
O8	2.5033890387	0.0327346495	0.0473210116
C9	1.4280127611	-2.0988357086	0.0718718098
C10	0.3340748761	-2.9465881764	0.4847615676
C11	0.4299134232	-4.3171025624	0.4763186120
C12	1.6487074626	-4.9382021483	0.0682004457
H13	1.2217328065	1.8850070352	0.3859350082
H14	-0.7497493897	3.4052659039	0.3644183900
H15	-3.0485513840	2.4944049606	-0.1118186982
H16	-3.2528881726	0.0355031053	-0.6297590766
H17	-1.3271689437	-1.4171456730	-0.6068886000
H18	-0.5667571147	-2.4915752682	0.8793022950
H19	-0.4088659364	-4.9181075255	0.8344248711
H20	1.7923687482	-6.0163732401	0.0606608800
N21	2.6644063513	-2.7328874794	-0.1822579319
C23	2.7064635954	-4.0502137899	-0.1879576746
H24	3.6961362936	-4.4821483056	-0.4097962638

#####mol64#####

#####mol#####

23

structure

C1	0.9870175719	1.6437343827	0.0845896258
C2	0.9338928936	2.9202522137	-0.4956197946
N3	-0.1467637076	3.6981038519	-0.4891750044
C4	-1.2345329316	3.2313631887	0.1353452265
C5	-1.2895687453	1.9900989348	0.7633252409
C6	-0.1606669587	1.1785456180	0.7317712245
C7	2.2910673467	0.9020113737	0.0516858459
O8	3.3367708987	1.5273959429	0.0459663690
C9	2.3061725111	-0.5972386975	0.0279639332
C10	1.2771259075	-1.3608667268	-0.5375510708
C11	1.3807541586	-2.7486499313	-0.5918176439
C12	2.5035930624	-3.3855923499	-0.0695169247
C13	3.5356229751	-2.6316569046	0.4907560153
C14	3.4433164997	-1.2468701728	0.5271809881
H15	1.8190459393	3.3111982041	-0.9864487762
H16	-2.1004375960	3.8873938032	0.1371286527
H17	-2.1936329395	1.6711142828	1.2679140898
H18	-0.1645251659	0.2123953014	1.2219202828
H19	0.4086472712	-0.8728355803	-0.9625165288
H20	0.5867184892	-3.3309682443	-1.0449318358
H21	2.5788627760	-4.4665217341	-0.1047506732
H22	4.4130212494	-3.1259268180	0.8916470430
H23	4.2440851282	-0.6429675229	0.9355573683

#####mol\_reduced#####

23

structure

C1	0.9669361170	1.6171110935	0.0675989283
C2	1.0151422979	3.0023715517	-0.2702137040
N3	-0.0162367511	3.8373869731	-0.2663178664
C4	-1.2150944891	3.3493969747	0.1132572636
C5	-1.3862638558	2.0239148490	0.5156486346
C6	-0.3031729672	1.1565288139	0.4981987433
C7	2.2243127749	0.8631399319	0.0299398993
O8	3.3240758913	1.4992622207	0.0009876267
C9	2.2598690405	-0.6118195944	0.0292859151
C10	1.2013207449	-1.4762390029	-0.3481512135
C11	1.3592999295	-2.8566976932	-0.3644066274
C12	2.5764823000	-3.4480307480	-0.0094481793
C13	3.6457066631	-2.6107881511	0.3356598253
C14	3.4969015292	-1.2340910482	0.3438785624
H15	1.9816745020	3.4064019608	-0.5519727234
H16	-2.0491022247	4.0475001024	0.1045482883
H17	-2.3595041388	1.6801977609	0.8564722067
H18	-0.4264881160	0.1435317650	0.8594124948
H19	0.2589655224	-1.0592522368	-0.6796670252
H20	0.5251970018	-3.4815083302	-0.6743482551
H21	2.6938569823	-4.5269507382	-0.0182607133
H22	4.6074655296	-3.0455806480	0.5975318680
H23	4.3235306822	-0.5774080801	0.5850903395

#####mol\_double\_reduced#####

23

structure

C1	0.9584808147	1.5907476608	0.0728679732
C2	1.0509996485	3.0288049923	-0.1061897038
N3	0.0507052597	3.8937161749	-0.1427330532
C4	-1.2140052202	3.4169802935	0.0437018238
C5	-1.4386693896	2.0594751767	0.3314474207
C6	-0.3885619932	1.1585418039	0.3607042887
C7	2.1966695055	0.8446222317	0.0471223518
O8	3.3305106740	1.4958399231	0.0324081171
C9	2.2295862384	-0.6065024367	0.0356712388
C10	1.1586489164	-1.5418016828	-0.2011968154
C11	1.3537241707	-2.9133801865	-0.2027863162
C12	2.6224430086	-3.4934128600	0.0211808474
C13	3.7037047850	-2.5983220143	0.1923669142
C14	3.5268020423	-1.2304235632	0.1840207211
H15	2.0595100747	3.4153858348	-0.2222139265
H16	-2.0295184843	4.1393107245	-0.0060805952
H17	-2.4498739344	1.7175074047	0.5660609434
H18	-0.5863342810	0.1411283015	0.6742015083
H19	0.1721432727	-1.1746093743	-0.4544371737
H20	0.4974021671	-3.5601074094	-0.4089167391
H21	2.7642103679	-4.5720576186	0.0292498564
H22	4.7115981867	-2.9999086865	0.3290334082
H23	4.3560242295	-0.5399908682	0.2890349939

#####mol65#####

#####mol#####

23

structure

C1	1.0436431015	1.6742223947	0.1685102835
C2	1.0123234402	2.9544003674	-0.3905415645
C3	-0.1606290789	3.6954483167	-0.3086862611
N4	-1.2697192960	3.2641425654	0.3035597927
C5	-1.2252804954	2.0515244207	0.8589916461
C6	-0.1084252746	1.2181624031	0.8132567368
C7	2.3385078301	0.9035294947	0.1318173523
O8	3.3908836028	1.5147084240	0.1633080900
C9	2.3274979345	-0.5920320612	0.0620964889
C10	1.2806295843	-1.3188667453	-0.5193735282
C11	1.3606996961	-2.7054997956	-0.6201271613
C12	2.4767179767	-3.3778396099	-0.1284251024
C13	3.5256962643	-2.6605726395	0.4484561355
C14	3.4573926772	-1.2766254677	0.5311714777
H15	1.8963088989	3.3528462286	-0.8719037258
H16	-0.2142843655	4.6863291657	-0.7501232526
H17	-2.1280172531	1.7243137642	1.3672252241
H18	-0.1373944429	0.2482403768	1.2936256679
H19	0.4160634351	-0.8028383427	-0.9179858943

H20	0.5530186503	-3.2592550590	-1.0846196035
H21	2.5332816074	-4.4580814607	-0.1998130539
H22	4.3971259498	-3.1826672515	0.8262262824
H23	4.2708779945	-0.7001772977	0.9537317563

#####mol\_reduced#####

23

structure

C1	1.0301214327	1.6472016526	0.1242517375
C2	1.0908017105	3.0413452290	-0.1584499580
C3	-0.0392293919	3.8277032771	-0.0692223139
N4	-1.2638238255	3.3925510281	0.3016369851
C5	-1.3156408551	2.0822585329	0.6116529026
C6	-0.2517153526	1.1981206283	0.5449543234
C7	2.2664353828	0.8730713323	0.0452090063
O8	3.3775965823	1.4837295354	-0.0228104354
C9	2.2816655273	-0.6080304928	0.0532633225
C10	1.2147011072	-1.4536173354	-0.3308529441
C11	1.3518490883	-2.8374448216	-0.3420261576
C12	2.5567286248	-3.4434725476	0.0245360547
C13	3.6347353853	-2.6234210999	0.3783607677
C14	3.5047978096	-1.2436498964	0.3809972747
H15	2.0484109370	3.4581788219	-0.4436691833
H16	0.0263237950	4.8895532056	-0.3080365509
H17	-2.2864326114	1.7171168783	0.9480984888
H18	-0.4088597530	0.1766719057	0.8661798750
H19	0.2822523925	-1.0208977406	-0.6690594323
H20	0.5116756524	-3.4511200639	-0.6569329565
H21	2.6587036150	-4.5241136372	0.0182406621
H22	4.5871635772	-3.0721273180	0.6500140476
H23	4.3386537782	-0.5974634845	0.6258315087

#####mol\_double\_reduced#####

23

structure

C1	1.0217716919	1.6161254826	0.1233445874
C2	1.1218950385	3.0543982807	-0.0321797964
C3	0.0149998787	3.8665846268	-0.0051251125
N4	-1.2783739319	3.4740128124	0.1961662402
C5	-1.3708072181	2.1323570233	0.4188262860
C6	-0.3399507488	1.2155784235	0.4005234002
C7	2.2402242111	0.8526754211	0.0766308719
O8	3.3863093229	1.4802410895	0.0403794363
C9	2.2543308200	-0.6037790307	0.0773239796
C10	1.1753418145	-1.5229725410	-0.1621305611
C11	1.3518749066	-2.8975801007	-0.1565637225
C12	2.6127485562	-3.4901348724	0.0733292911
C13	3.7023504605	-2.6106111285	0.2503227482
C14	3.5409710936	-1.2393582462	0.2376907993
H15	2.1200803148	3.4517820528	-0.1767358557
H16	0.1490241084	4.9451288877	-0.1526702054

H17	-2.3799243897	1.7698239722	0.6471943254
H18	-0.5797503019	0.1936287375	0.6674854510
H19	0.1952081446	-1.1419054560	-0.4173014501
H20	0.4890327446	-3.5346730740	-0.3628823208
H21	2.7423469850	-4.5703099354	0.0791652874
H22	4.7038531217	-3.0242893421	0.3951304058
H23	4.3759535753	-0.5565937426	0.3456974893

#####mol66#####

#####mol#####

23

structure

C1	1.0726463679	1.7124060836	0.1760178796
C2	1.0339886669	3.0064304256	-0.3552918547
C3	-0.1164492508	3.7639874242	-0.2018901608
C4	-1.1866989749	3.2108767904	0.5017852604
N5	-1.1620713977	1.9921926177	1.0466409188
C6	-0.0535574597	1.2660009076	0.8779808143
C7	2.3473931479	0.9280651063	0.0587187585
O8	3.4076124451	1.5243992446	-0.0238256919
C9	2.3206660856	-0.5698682512	0.0459083476
C10	1.2400058918	-1.3085974700	-0.4519377343
C11	1.3040586580	-2.6986800070	-0.5039322370
C12	2.4389044264	-3.3627395682	-0.0458419530
C13	3.5220423753	-2.6339366141	0.4473182370
C14	3.4684736936	-1.2471803034	0.4800987399
H15	1.9064320738	3.3882049618	-0.8714309764
H16	-0.1897011485	4.7644231368	-0.6111908623
H17	-2.1048310271	3.7753341419	0.6390475933
H18	-0.0551423180	0.2878795929	1.3478351035
H19	0.3592535681	-0.8009426365	-0.8247497952
H20	0.4684726782	-3.2615565522	-0.9034612283
H21	2.4830650351	-4.4455162726	-0.0779069090
H22	4.4080596734	-3.1495305177	0.7995243991
H23	4.3075318633	-0.6632109126	0.8371146017

#####mol\_reduced#####

23

structure

C1	1.0507763265	1.6897281754	0.1584485640
C2	1.1249058150	3.0727523166	-0.1629512484
C3	0.0013172509	3.8720646202	-0.0581690995
C4	-1.1981575563	3.3137192586	0.3928129353
N5	-1.2966285923	2.0214375538	0.7613736168
C6	-0.2122678575	1.2582444418	0.6457358908
C7	2.2822667974	0.8976882475	0.0684755077
O8	3.3922833490	1.5096109212	-0.0214578646
C9	2.2873067382	-0.5772974822	0.0767716174
C10	1.1990458086	-1.4210634146	-0.2581916628
C11	1.3282764677	-2.8044517406	-0.2705114691
C12	2.5456145742	-3.4183350633	0.0431815562



C13	3.6430753193	-2.6017773528	0.3451374216
C14	3.5220889518	-1.2221606200	0.3503239629
H15	2.0855707094	3.4578071984	-0.4809377108
H16	0.0450691317	4.9275469442	-0.3157436580
H17	-2.0997786992	3.9149327478	0.4869079239
H18	-0.3318347463	0.2395967217	0.9996904313
H19	0.2535774326	-0.9867485552	-0.5558851426
H20	0.4707164793	-3.4135894237	-0.5449988521
H21	2.6408684815	-4.4994873699	0.0357122752
H22	4.6045993705	-3.0547745504	0.5751591932
H23	4.3695713576	-0.5807865014	0.5576861075

#####mol\_double\_reduced#####

23

structure

C1	1.0356531192	1.6645271333	0.1578660773
C2	1.1705891811	3.0969159096	-0.0182678507
C3	0.0648617549	3.9195855629	0.0202984353
C4	-1.2114417908	3.3867151533	0.2738966423
N5	-1.3770030956	2.0604152702	0.5448134094
C6	-0.3103599937	1.2708519200	0.4886900257
C7	2.2483876200	0.8766236009	0.1005135272
O8	3.3912888676	1.5108829808	0.0427513160
C9	2.2592735745	-0.5728577098	0.1019908089
C10	1.1721877657	-1.4958678653	-0.1073414034
C11	1.3478194206	-2.8693357553	-0.1013998432
C12	2.6138660702	-3.4662332052	0.0966874514
C13	3.7092323416	-2.5849824273	0.2407212797
C14	3.5509214252	-1.2144642814	0.2290064181
H15	2.1791939180	3.4595262969	-0.1755461004
H16	0.1755440555	4.9970426526	-0.1324186911
H17	-2.1014101624	4.0153806158	0.3212756916
H18	-0.5068820082	0.2415868647	0.7737848928
H19	0.1843187863	-1.1172529991	-0.3362570833
H20	0.4778152197	-3.5048814695	-0.2824461719
H21	2.7419885067	-4.5465475346	0.1009302659
H22	4.7145695576	-2.9989092554	0.3587956326
H23	4.3920041921	-0.5360443625	0.3143426509

#####mol67#####

#####mol#####

23

structure

C1	1.0096458115	1.7329992552	0.1366659112
C2	1.0921049006	3.0861207390	-0.2118304620
C3	-0.0517312742	3.8677464965	-0.1302712633
C4	-1.2342067124	3.2796777622	0.3100868806
C5	-1.2175320757	1.9268900832	0.6406262835
N6	-0.1275657412	1.1620681203	0.5530994009
C7	2.2872200676	0.9182761891	0.0932062934
O8	3.3443089663	1.5268429019	0.0594208120

C9	2.2838358114	-0.5791207562	0.0990377034
C10	1.1857186250	-1.3695957972	-0.2668638246
C11	1.3021894285	-2.7564777635	-0.3001901050
C12	2.5031113469	-3.3705649229	0.0453636581
C13	3.6009322461	-2.5920314086	0.4134649389
C14	3.4940936560	-1.2085996170	0.4296145196
H15	2.0451911498	3.4890672126	-0.5260480731
H16	-0.0220581674	4.9175484631	-0.3988759314
H17	-2.1502537851	3.8515093432	0.3975466246
H18	-2.1195371114	1.4336421513	0.9917801691
H19	0.2459635155	-0.9011431360	-0.5153865893
H20	0.4493957500	-3.3584423029	-0.5928167518
H21	2.5857926518	-4.4516589612	0.0261174007
H22	4.5386188875	-3.0654155534	0.6816098552
H23	4.3408600472	-0.5874898104	0.6928200930

#####mol\_reduced#####

23

structure

C1	1.0060866883	1.7017366147	0.1324867939
C2	1.1476288225	3.1237353991	0.1286080491
C3	0.0362460553	3.9325652238	0.1313538600
C4	-1.2463886168	3.3481570217	0.1379038031
C5	-1.3016850963	1.9548589471	0.1411811552
N6	-0.2470126667	1.1466631823	0.1386655914
C7	2.2327905285	0.9068812851	0.1300036955
O8	3.3466092083	1.5208578760	0.1250750256
C9	2.2559604701	-0.5791633348	0.1333906957
C10	1.1380368906	-1.4466213050	0.1360507447
C11	1.3016705844	-2.8282960514	0.1385184876
C12	2.5727980788	-3.4084182348	0.1386464047
C13	3.6892410053	-2.5661068780	0.1361159596
C14	3.5348592420	-1.1879769948	0.1334006882
H15	2.1550946967	3.5171364178	0.1237116425
H16	0.1473960689	5.0144415344	0.1284507546
H17	-2.1533177555	3.9428479714	0.1404707128
H18	-2.2735383487	1.4571426625	0.1461592519
H19	0.1512222348	-1.0084178732	0.1361525891
H20	0.4193941875	-3.4641284852	0.1402018218
H21	2.6910542396	-4.4880767936	0.1406545256
H22	4.6895244654	-2.9930913949	0.1363173704
H23	4.3893377938	-0.5229800976	0.1312858212

#####mol\_double\_reduced#####

23

structure

C1	1.0164362620	1.6708862120	0.1338735896
C2	1.1458473087	3.1183306754	0.1252398932
C3	0.0487931840	3.9349611153	0.1293930741
C4	-1.2625012456	3.3696829071	0.1416813636
C5	-1.3108418775	1.9646081003	0.1529275441

N6	-0.2839825645	1.1360197795	0.1496312652
C7	2.2311539620	0.9073627865	0.1264019803
O8	3.3816996978	1.5341376745	0.1146938286
C9	2.2446585268	-0.5533522935	0.1312632961
C10	1.1311115479	-1.4574883975	0.1426418051
C11	1.3036645389	-2.8328357795	0.1460400282
C12	2.5843814471	-3.4298862586	0.1377522658
C13	3.6925365632	-2.5614098484	0.1258300987
C14	3.5370628628	-1.1863948699	0.1236444666
H15	2.1631893826	3.4912679610	0.1161664064
H16	0.1775623549	5.0207711146	0.1223639635
H17	-2.1687746182	3.9706127854	0.1496283552
H18	-2.2990110793	1.4801548552	0.1657857655
H19	0.1391576045	-1.0264513430	0.1494062657
H20	0.4168706847	-3.4711188747	0.1528863230
H21	2.7078089070	-4.5117210423	0.1371750216
H22	4.7020227029	-2.9817883082	0.1179854533
H23	4.3819460906	-0.5068354117	0.1140422298

#####mol68#####

#####mol#####

22

structure

C1	2.3214675130	-0.5915162892	-0.0518981427
C2	2.3297048206	0.9229697009	0.0142193336
O3	3.3671018427	1.5379881990	0.0190417810
C4	0.9987167862	1.6471673963	0.0749175396
C5	-0.0478821207	1.1677985431	0.8678285644
C6	-1.2075006622	1.9299771210	0.9776759803
C7	-1.2880316308	3.1236113910	0.2717901681
C8	-0.1953653404	3.5080463680	-0.5073586862
N9	0.9296856887	2.8024768691	-0.6004339345
H10	0.0523510494	0.2299993368	1.4003420618
H11	-2.0290029692	1.5960891731	1.6011543610
H12	-2.1719582428	3.7482537394	0.3192462516
H13	-0.2274822335	4.4309998375	-1.0798671721
C14	1.3589875435	-1.2771586663	-0.7986189167
H15	0.5611709877	-0.7371568660	-1.2933164117
N16	3.3324478254	-1.2105085983	0.5739814307
C17	3.4040301591	-2.5359038306	0.4757064134
H18	4.2250856432	-3.0097372934	1.0068035753
C19	2.5019023471	-3.3076099425	-0.2595672351
H20	2.6200046775	-4.3832669983	-0.3131261878
C21	1.4611623617	-2.6609419359	-0.9137323718
H22	0.7417866659	-3.2190046392	-1.5020623466

#####mol\_reduced#####

22

structure

C1	2.3085889970	-0.5758041396	-0.0270447420
C2	2.3006594007	0.9045248944	0.0019040589

O3	3.3762925024	1.5434106918	-0.0062841031
C4	1.0071520142	1.6295830020	0.0397284162
C5	-0.1685069034	1.1008249196	0.6360553767
C6	-1.3161381047	1.8646254474	0.7252932103
C7	-1.3055377959	3.1755673155	0.2223073001
C8	-0.1035108544	3.6292777289	-0.3226146242
N9	1.0135314682	2.9183028632	-0.4170645399
H10	-0.1508631464	0.1037819584	1.0578843711
H11	-2.2061264636	1.4588173147	1.1991488459
H12	-2.1774653856	3.8190882408	0.2689904344
H13	-0.0449421667	4.6481913933	-0.7113644801
C14	1.2519820832	-1.3562606738	-0.5694402859
H15	0.3716402937	-0.8639854626	-0.9630198221
N16	3.4589074010	-1.1907412950	0.3872894988
C17	3.5354457992	-2.5129282128	0.3054067895
H18	4.4722140385	-2.9507667005	0.6571719906
C19	2.5329429603	-3.3517637420	-0.1840727752
H20	2.6711827878	-4.4268522005	-0.2225093141
C21	1.3601625467	-2.7310223422	-0.6448359453
H22	0.5540189421	-3.3183085390	-1.0767570413

#####mol\_double\_reduced#####

22

structure

C1	2.3021808977	-0.5562483812	-0.0231428243
C2	2.3049623752	0.9083542642	-0.0124175127
O3	3.4028310932	1.5552517117	-0.0393517914
C4	1.0236848441	1.6165762058	0.0302369578
C5	-0.2110842851	1.0817533270	0.5364447109
C6	-1.3637152251	1.8308050520	0.5970036137
C7	-1.3395085775	3.1910203126	0.1673072540
C8	-0.0807520317	3.6696924673	-0.2208864571
N9	1.0468936855	2.9854796181	-0.2903279435
H10	-0.2221726395	0.0740209759	0.9345561641
H11	-2.2712010335	1.3947574127	1.0183726034
H12	-2.2089498978	3.8430035475	0.2140671942
H13	0.0030037749	4.7329417235	-0.4963829131
C14	1.2187228742	-1.3875175257	-0.4726860316
H15	0.3179556674	-0.9172600909	-0.8489850436
N16	3.5217289996	-1.1928349818	0.2668403353
C17	3.5716675605	-2.5118769604	0.2247350486
H18	4.5519520580	-2.9480800370	0.4740800147
C19	2.5298091450	-3.3888242574	-0.1063507008
H20	2.6774946931	-4.4661205477	-0.1348168546
C21	1.3134146743	-2.7597926665	-0.5063861623
H22	0.4778009360	-3.3510248077	-0.8850469196

#####mol69#####

#####mol#####

22

structure

C1	0.9837797043	1.6567517774	0.0467404931
N2	0.9884988170	2.8380364893	0.6783217286
C3	-0.1338129198	3.5545317712	0.6592030030
C4	-1.2961661161	3.1542695578	-0.0014966349
C5	-1.2915469578	1.9330780608	-0.6634163269
C6	2.3102801847	0.9235575315	0.0175326001
O7	3.3328341501	1.5336079156	-0.2087523065
C8	2.3302738469	-0.5575603544	0.2454726714
C9	1.3453123762	-1.2475465403	0.9570348531
H10	-0.1038910840	4.4999868505	1.1935154775
H11	-2.1746028843	3.7881198096	0.0058304340
H12	-2.1692172675	1.5860089575	-1.1964727942
H13	0.4871258629	-0.7241246090	1.3616856983
C14	1.4970165025	-2.6146714431	1.1600888565
H15	0.7627063258	-3.1830328184	1.7179326037
C16	2.6218813622	-3.2437314785	0.6337342480
H17	2.7687068826	-4.3114010948	0.7702152172
N18	3.5776845290	-2.6039550933	-0.0514062601
C20	3.4295542766	-1.2922557031	-0.2245648642
H21	4.2130847967	-0.7736630053	-0.7667640096
C22	-0.1343527945	1.1600279199	-0.6289768204
H23	-0.0913565755	0.2024239844	-1.1334549764

#####mol\_reduced#####

22

structure

C1	0.9979682037	1.6578698666	0.0959480843
N2	1.0588349536	2.9890594437	0.4146710164
C3	-0.0550646604	3.7062190180	0.3491897209
C4	-1.3074755028	3.2233069617	-0.0356816868
C5	-1.3744454259	1.8700023627	-0.4073871596
C6	2.2682094900	0.9130776576	0.1202458045
O7	3.3675663234	1.5203381016	0.0172219443
C8	2.2783845929	-0.5596769227	0.2568150381
C9	1.2628431334	-1.3772725423	0.8034261952
H10	0.0486051100	4.7583291794	0.6235891077
H11	-2.1743463816	3.8743726581	-0.0649775482
H12	-2.3054917359	1.4377086888	-0.7646162167
H13	0.3444705766	-0.9367825994	1.1717954428
C14	1.4594023338	-2.7472060504	0.9167624810
H15	0.6880400578	-3.3812286114	1.3455754692
C16	2.6675418350	-3.3031684884	0.4953860081
H17	2.8468044399	-4.3739853559	0.5632568447
N18	3.6735824151	-2.5552983761	0.0038985532
C20	3.4753777692	-1.2444357312	-0.0916036651
H21	4.2981144206	-0.6422377077	-0.4617928446
C22	-0.2330928066	1.0960682182	-0.3418506785
H23	-0.2644701140	0.0664672539	-0.6744001639

#####mol\_double\_reduced#####

22

structure

C1	1.0135781732	1.6483174161	0.0802404455
N2	1.0928017635	3.0495153645	0.2157395610
C3	-0.0263128105	3.7471039057	0.2045334184
C4	-1.3313886131	3.2585820783	0.0334373206
C5	-1.4198339444	1.8620660734	-0.2425309173
C6	2.2583296501	0.9085080507	0.1203760322
O7	3.3971503447	1.5088085705	0.0372807875
C8	2.2459105058	-0.5494636120	0.2548743190
C9	1.2070691638	-1.4403896556	0.6940688995
H10	0.1022966287	4.8338717210	0.3336362673
H11	-2.1950672547	3.9194425146	0.0373146448
H12	-2.3738962130	1.4074880690	-0.5173085058
H13	0.2516995388	-1.0495447819	1.0232098089
C14	1.4333591041	-2.8039839808	0.7797034628
H15	0.6368993768	-3.4649807070	1.1286307234
C16	2.6935011258	-3.3388272383	0.4613023216
H17	2.8919358343	-4.4103167266	0.5065042529
N18	3.7358492054	-2.5301900169	0.1271884902
C20	3.5095088387	-1.2262966712	0.0555490052
H21	4.3492331974	-0.5767519091	-0.1732391440
C22	-0.2812955779	1.0923864887	-0.2256191742
H23	-0.3541030882	0.0517813777	-0.5188014226

#####mol70#####

#####mol#####

22

structure

C1	2.3003916920	-1.1518992097	0.0912836367
N2	3.2656871959	-1.7508750054	-0.6186866061
C3	3.3293715578	-3.0801699469	-0.5784748464
C4	2.4671963372	-3.8731874304	0.1808807084
C5	1.4759066355	-3.2453667430	0.9242566735
C6	2.3294420482	0.3618353665	0.0862486586
O7	3.3843179070	0.9502094830	0.1701028832
C8	1.0351244127	1.1265433407	-0.0024685926
C9	1.0074870284	2.4498617667	0.4458840368
C10	-0.1717562347	3.1748130912	0.3260108951
N11	-1.2921923635	2.6839245728	-0.2180497012
C12	-1.2531826340	1.4269773757	-0.6644569871
C13	-0.1283140760	0.6081918153	-0.5751041354
C14	1.3789236821	-1.8575918286	0.8698216555
H15	4.1114076479	-3.5377380852	-1.1780332466
H16	2.5776325739	-4.9509153284	0.1851495558
H17	0.7893157944	-3.8209769801	1.5342896143
H18	1.8999614354	2.8893270665	0.8729072726
H19	-0.2232741631	4.2006230611	0.6791121810
H20	-2.1666591091	1.0511186296	-1.1166822799
H21	-0.1630415845	-0.4011570495	-0.9653790230
H22	0.6185527269	-1.3323254342	1.4343004041

#####mol\_reduced#####

22

structure

C1	2.3022200350	-1.1406724232	0.0513678854
N2	3.4302987032	-1.7425675309	-0.4267097384
C3	3.5083774814	-3.0672230765	-0.3842889681
C4	2.5257240826	-3.9148320448	0.1288867966
C5	1.3787889449	-3.3061377750	0.6580691114
C6	2.2874873146	0.3389703680	0.0535859029
O7	3.3742951786	0.9754067361	0.0930551321
C8	1.0190044939	1.0820899707	0.0133294060
C9	1.0511914181	2.4738779836	0.2948549411
C10	-0.1019525793	3.2306810179	0.2324318639
N11	-1.3209379410	2.7610928503	-0.1072661500
C12	-1.3474907609	1.4501316552	-0.4137074582
C13	-0.2565992009	0.5967571609	-0.3749059964
C14	1.2684981457	-1.9288612217	0.6196911882
H15	4.4266886260	-3.4966263839	-0.7894600475
H16	2.6612710234	-4.9910742050	0.1315826266
H17	0.5926990667	-3.9032053794	1.1125545760
H18	2.0048209210	2.9155976247	0.5552987604
H19	-0.0595883940	4.2940421993	0.4687325985
H20	-2.3169375540	1.0587756366	-0.7227256318
H21	-0.3920088711	-0.4315741908	-0.6859013374
H22	0.4097326422	-1.4444638309	1.0656085064

#####mol\_double\_reduced#####

22

structure

C1	2.3070658521	-1.1236508555	0.0487817507
N2	3.5308222178	-1.7431673618	-0.2560169617
C3	3.5872968072	-3.0622719262	-0.2581016809
C4	2.5490294944	-3.9539524968	0.0472304838
C5	1.3350197816	-3.3445733503	0.4752508590
C6	2.2796142790	0.3294115957	0.0423846853
O7	3.3743144011	1.0105328539	0.0397196116
C8	1.0092851422	1.0428385274	0.0256464989
C9	1.0616483749	2.4776348884	0.1894560528
C10	-0.0732515456	3.2532962965	0.1653521213
N11	-1.3482341326	2.8159840838	-0.0404336362
C12	-1.3969622568	1.4734616390	-0.2677574609
C13	-0.3315215592	0.5951086429	-0.2536427712
C14	1.2289496061	-1.9734770562	0.4811500806
H15	4.5693131126	-3.4853777618	-0.5211479985
H16	2.6968217067	-5.0311704463	0.0273429159
H17	0.5063251796	-3.9518042762	0.8436354688
H18	2.0477106716	2.9050779487	0.3315375866
H19	0.0226112689	4.3346029943	0.3186809950
H20	-2.3926272497	1.0779780490	-0.4969535569
H21	-0.5315983086	-0.4358795380	-0.5208654699

H22 0.3319071614 -1.5217138989 0.8853396776

#####mol71#####

#####mol#####

22

structure

C1	0.9710112889	1.1150493174	0.1061879390
C2	0.9280570375	2.3936435002	-0.4702175155
N3	-0.1507871410	3.1737411147	-0.4718474197
C4	-1.2464558652	2.7075250771	0.1392226210
C5	-1.3120479636	1.4635780096	0.7611139836
C6	2.2690620796	0.3663090162	0.0774638423
O7	3.3233319499	0.9751054540	0.0556344219
C8	2.2678949976	-1.1324788219	0.0754095959
C9	3.3733650086	-1.7988126869	0.6257850542
N10	3.5100472904	-3.1229353243	0.6465013230
C11	2.5379667353	-3.8493520773	0.0819859186
C12	1.4066951607	-3.2952149434	-0.5109198694
C13	1.2656438091	-1.9119894870	-0.5082309744
C14	-0.1850496821	0.6495923564	0.7383165720
H15	1.8189239592	2.7833811413	-0.9515849427
H16	-2.1105766523	3.3658857970	0.1344389755
H17	-2.2224004173	1.1453611867	1.2545441499
H18	4.1723736943	-1.2136816038	1.0689844713
H19	2.6765485157	-4.9266491618	0.1012711813
H20	0.6594274969	-3.9331327197	-0.9671228047
H21	0.4051259424	-1.4477782892	-0.9749325470
H22	-0.1974059901	-0.3177614812	1.2260496104

#####mol\_reduced#####

22

structure

C1	0.9400758604	1.0830343040	0.1056975443
C2	0.9914681568	2.4628474506	-0.2443488923
N3	-0.0411815975	3.2976163427	-0.2536360309
C4	-1.2400947309	2.8119327157	0.1244331239
C5	-1.4139805325	1.4907447637	0.5374307278
C6	2.1993156750	0.3254979743	0.0808629082
O7	3.2985347669	0.9608874954	0.0562447797
C8	2.2244296743	-1.1433979200	0.0796139681
C9	3.4594280696	-1.7839601991	0.3873485901
N10	3.6663628961	-3.0951926117	0.4100624168
C11	2.6305058280	-3.8967357732	0.0915642129
C12	1.3823070181	-3.3929553886	-0.2752325449
C13	1.1744247895	-2.0205416856	-0.2850324265
C14	-0.3293305013	0.6243687514	0.5324088486
H15	1.9590915067	2.8648989419	-0.5248443131
H16	-2.0747847323	3.5092305293	0.1046051880
H17	-2.3889412415	1.1496995479	0.8752906433
H18	4.3027668949	-1.1427234390	0.6202045536
H19	2.8178300254	-4.9678018325	0.1218781735



H20	0.5850471010	-4.0719844872	-0.5656311762
H21	0.2212053650	-1.6298550623	-0.6176467035
H22	-0.4543313853	-0.3863490870	0.8995533825

#####mol\_double\_reduced#####

22

structure

C1	0.9316133543	1.0556459748	0.1134543550
C2	1.0193991514	2.4921249173	-0.0628909839
N3	0.0157556932	3.3543214270	-0.0873927346
C4	-1.2446653311	2.8716585625	0.1080814574
C5	-1.4639754319	1.5127540562	0.3886563819
C6	2.1727971582	0.3102942949	0.0746616849
O7	3.3038425407	0.9623075178	0.0416304535
C8	2.1948776795	-1.1381478043	0.0712812640
C9	3.4894660410	-1.7778568293	0.2017168447
N10	3.7351191721	-3.0776676204	0.2425699831
C11	2.6788922041	-3.9307351011	0.1146246538
C12	1.3803823306	-3.4459861888	-0.1139991015
C13	1.1290703441	-2.0847603321	-0.1449125222
C14	-0.4104060471	0.6146224375	0.4020745275
H15	2.0253981370	2.8823610621	-0.1874107699
H16	-2.0629481277	3.5913378315	0.0679939696
H17	-2.4727460095	1.1661588119	0.6254545480
H18	4.3353221825	-1.1000999714	0.2719487884
H19	2.8944129725	-4.9983947182	0.1679401403
H20	0.5652580203	-4.1504502352	-0.2959092569
H21	0.1349717681	-1.7460921483	-0.4080943617
H22	-0.6024260991	-0.4065363803	0.7064299048

#####mol72#####

#####mol#####

22

structure

C1	2.2891349655	-1.1224422971	0.0740607571
C2	3.3664172961	-1.8301827864	-0.4813067460
N3	3.4862471837	-3.1551942766	-0.4401788749
C4	2.5263923316	-3.8390107864	0.1944076971
C5	1.4234405197	-3.2407059066	0.7978859412
C6	2.3083198899	0.3722665796	-0.0007487230
O7	3.3653463157	0.9710438001	-0.0639579574
C8	1.0152322386	1.1436553820	-0.0017131803
C9	1.0101094060	2.4390819731	0.5219763509
C10	-0.1679192550	3.1753847176	0.4797083886
N11	-1.3057697095	2.7237172543	-0.0610041891
C12	-1.2875140115	1.4956743519	-0.5829304160
C13	-0.1671875258	0.6661440650	-0.5715873915
C14	1.2982916172	-1.8577433225	0.7306908858
H15	4.1553199732	-1.2789829590	-0.9822093964
H16	2.6514587713	-4.9176188627	0.2246126319
H17	0.6850267766	-3.8449105265	1.3106845791

H18	1.9164186454	2.8513445501	0.9467332984
H19	-0.2022505718	4.1784581235	0.8945804881
H20	-2.2145987096	1.1529578092	-1.0336148593
H21	-0.2186941056	-0.3163996987	-1.0236313865
H22	0.4591566520	-1.3592844889	1.2007401053

#####mol\_reduced#####

22

structure

C1	2.2470880882	-1.1349744524	0.0773135433
C2	3.4511326283	-1.7893145894	-0.2995794610
N3	3.6438411719	-3.1046093070	-0.3144109039
C4	2.6242248819	-3.8867376821	0.0847126801
C5	1.4077039571	-3.3658998616	0.5230311465
C6	2.2355722890	0.3405641568	0.0619197031
O7	3.3467889677	0.9534408579	0.0653893599
C8	0.9916730474	1.1103048882	0.0316519832
C9	1.0605841771	2.5077749436	0.2850699906
C10	-0.0776941602	3.2871055897	0.2403720276
N11	-1.3161322529	2.8374377557	-0.0568343042
C12	-1.3780448678	1.5222432251	-0.3381643687
C13	-0.3060268625	0.6449926007	-0.3101345391
C14	1.2157510310	-1.9900013770	0.5235266614
H15	4.2844477508	-1.1612368987	-0.5955145676
H16	2.7992086840	-4.9602027550	0.0626881670
H17	0.6249263272	-4.0316110081	0.8757610633
H18	2.0293366516	2.9346594861	0.5115812623
H19	-0.0067060583	4.3534781098	0.4547861498
H20	-2.3632244162	1.1461858212	-0.6146670437
H21	-0.4738379825	-0.3834578574	-0.6025578886
H22	0.2911460462	-1.5798716384	0.9087043600

#####mol\_double\_reduced#####

22

structure

C1	2.2210925988	-1.1293733698	0.0683099724
C2	3.4987512536	-1.7785234823	-0.1357428690
N3	3.7318819333	-3.0825938293	-0.1671396177
C4	2.6834191371	-3.9214478102	0.0489412802
C5	1.4052062820	-3.4236429001	0.3509637756
C6	2.2091911522	0.3231478657	0.0436267624
O7	3.3499847346	0.9574219025	0.0225263117
C8	0.9814989413	1.0776854721	0.0286476610
C9	1.0756543828	2.5184107682	0.1387478614
C10	-0.0398400336	3.3198220083	0.1364919065
N11	-1.3356166596	2.9081282342	0.0048930799
C12	-1.4258702082	1.5606494582	-0.1712487509
C13	-0.3851333845	0.6539780888	-0.1697131776
C14	1.1690030781	-2.0592698891	0.3738588359
H15	4.3417497654	-1.1085683830	-0.2757646483
H16	2.8880900578	-4.9918044572	0.0076783461

H17	0.5991303751	-4.1174836684	0.5986698187
H18	2.0752762119	2.9280767748	0.2275718932
H19	0.0884022738	4.4031565631	0.2460711772
H20	-2.4407248034	1.1826062557	-0.3395097578
H21	-0.6254149979	-0.3789889342	-0.3895255638
H22	0.1960553971	-1.7046148986	0.6884461573

#####mol73#####

#####mol#####

22

structure

C1	2.2969311193	-1.1804442156	0.0551878370
C2	3.5300660671	-1.7851077709	-0.2138014550
C3	2.2394809682	0.3327764891	0.0448757728
O4	3.2920583394	0.9475949943	0.0143304433
C5	0.9432323472	1.0796096674	0.0918785738
N6	-0.0560965116	3.2303814305	0.5709649088
C7	-1.2355301889	2.7273812966	0.1865472112
C8	-1.4066574934	1.4195181785	-0.2563267638
C9	-0.3021920059	0.5762988029	-0.2991080897
N10	1.1975492590	-1.8818872687	0.3591728096
H11	4.3813361227	-1.1585374299	-0.4426089087
H12	-2.0810264109	3.4082636593	0.2341019457
H13	-2.3858957463	1.0684911513	-0.5592758349
H14	-0.3998754100	-0.4493397475	-0.6201847164
C15	3.6182422759	-3.1695127360	-0.1665619018
H16	4.5578113500	-3.6692539389	-0.3725647251
C17	2.4793042944	-3.9021020631	0.1560573335
H18	2.5014821611	-4.9838076548	0.2113083531
C19	1.2965384717	-3.2114223049	0.4100843438
H20	0.3883360660	-3.7491119379	0.6667786419
C21	0.9980421689	2.4196849718	0.5112576909
H22	1.9534883548	2.8347445018	0.8129326299

#####mol\_reduced#####

22

structure

C1	2.2605673751	-1.1692261004	0.0872929368
C2	3.5531046849	-1.7751368725	0.0783923175
C3	2.2038361841	0.2918969611	0.1178811435
O4	3.2976267811	0.9393938119	0.1360691054
C5	0.9359595724	1.0566578956	0.1292012931
N6	0.0180560446	3.3247709064	0.1771926257
C7	-1.2200109340	2.8026924049	0.1581153108
C8	-1.4553129869	1.4299003275	0.1248942084
C9	-0.3812963974	0.5477730956	0.1100617091
N10	1.1406975141	-1.9567821001	0.0678291632
H11	4.4073535690	-1.1118965440	0.0947386913
H12	-2.0450350797	3.5129628000	0.1703261720
H13	-2.4748572997	1.0535927973	0.1101730622
H14	-0.5261543572	-0.5220051089	0.0849981636

C15	3.6765147873	-3.1442110227	0.0505965496
H16	4.6615380168	-3.6047313753	0.0439566329
C17	2.5165388615	-3.9434862449	0.0309161429
H18	2.5615760878	-5.0267521116	0.0089362236
C19	1.2922958505	-3.2772649566	0.0411004463
H20	0.3665265246	-3.8553775190	0.0268465285
C21	1.0413641867	2.4720020341	0.1627099292
H22	2.0395541558	2.8945372091	0.1780219622

#####mol\_double\_reduced#####

22

structure

C1	2.2387284546	-1.1447492518	0.0891674913
C2	3.5465788360	-1.7743262194	0.0768838111
C3	2.2039589618	0.2906890794	0.1141439061
O4	3.3278804873	0.9611381814	0.1250842702
C5	0.9509638243	1.0343282758	0.1269755488
N6	0.0274313231	3.3316610056	0.1639168723
C7	-1.2278978476	2.8214549425	0.1563591455
C8	-1.4570151354	1.4343666818	0.1345956535
C9	-0.3954724771	0.5449963776	0.1199601151
N10	1.1112760827	-1.9830571933	0.0755277664
H11	4.3879543931	-1.0915259078	0.0884072558
H12	-2.0523785028	3.5370847052	0.1677962649
H13	-2.4823571308	1.0578692229	0.1290831535
H14	-0.5493625723	-0.5252144901	0.1029582900
C15	3.6843099233	-3.1349234092	0.0522087334
H16	4.6815646211	-3.5824946240	0.0432354478
C17	2.5254029666	-3.9684762933	0.0377327278
H18	2.5758811983	-5.0544327672	0.0194479307
C19	1.2948179800	-3.2903488520	0.0517592085
H20	0.3721450444	-3.8894948836	0.0421711014
C21	1.0428435274	2.4730736391	0.1499283494
H22	2.0500179838	2.8784188675	0.1558223162

#####mol74#####

#####mol#####

22

structure

C1	-0.0994930156	0.0234804177	0.0792041051
C2	-0.6402425993	-1.1232452225	-0.5225314986
N3	-1.9536087642	-1.3256347068	-0.6118029891
C4	-2.7342182143	-0.3641795375	-0.1103122627
C5	-2.2057338018	0.7778465328	0.4865076301
N6	-0.8905368487	0.9728313593	0.5892817506
C7	1.4049922148	0.1900448996	0.0740074102
C8	2.1074760252	1.1201976868	1.0100902219
O9	2.0358176444	-0.4690417624	-0.7357833780
C10	3.4397850128	1.4364622471	0.7005655789
C11	4.1848315202	2.2554178264	1.5364216189
C12	3.6153858174	2.7577941938	2.7071825730

C13	2.2995476423	2.4387111549	3.0318714622
C14	1.5432777501	1.6308873074	2.1873434710
H15	0.0183168817	-1.8786426772	-0.9337786612
H16	-3.8076701583	-0.5095027893	-0.1858128622
H17	-2.8528563248	1.5508391081	0.8899509836
H18	3.8693987856	1.0225560058	-0.2027950066
H19	5.2094882327	2.5001530431	1.2811693182
H20	4.1976879396	3.3938800266	3.3645437358
H21	1.8569863650	2.8229741215	3.9437389033
H22	0.5185019992	1.4036013007	2.4379547655

#####mol\_reduced#####

22

structure

C1	-0.0868718061	0.0418400183	0.0974666920
C2	-0.6458005364	-0.8736239034	-0.8506762864
N3	-1.9318311660	-1.1365017939	-0.9617398493
C4	-2.7508869792	-0.4709886604	-0.0981570525
C5	-2.2347586016	0.4209055098	0.8300338607
N6	-0.9378634112	0.6963798807	0.9543789750
C7	1.3587259935	0.2200705925	0.0897060942
C8	2.0776873784	1.1374755695	1.0209453951
O9	2.0499265376	-0.4334366291	-0.7491203169
C10	3.4827979416	1.1998044283	0.8788879528
C11	4.2622643433	2.0152279408	1.6860694884
C12	3.6725969821	2.8079488477	2.6749898480
C13	2.2861967092	2.7605192521	2.8313511532
C14	1.4976583209	1.9443888200	2.0248139618
H15	0.0396405469	-1.3820713183	-1.5195455069
H16	-3.8169075855	-0.6693185254	-0.1679611038
H17	-2.9070436610	0.9437204694	1.5127636199
H18	3.9224489203	0.5789813041	0.1083429269
H19	5.3402529616	2.0360722504	1.5462493964
H20	4.2804730294	3.4472232183	3.3084916669
H21	1.8086161845	3.3690192174	3.5953260779
H22	0.4257972985	1.9141803922	2.1518314057

#####mol\_double\_reduced#####

22

structure

C1	-0.0656062466	0.0583248037	0.1120992893
C2	-0.6424511789	-0.8671913996	-0.8436046313
N3	-1.9179855998	-1.1465918824	-0.9772422520
C4	-2.7673299058	-0.4769426291	-0.1100613957
C5	-2.2464176622	0.4233647614	0.8176714757
N6	-0.9673104030	0.7240636505	0.9725932474
C7	1.3592664510	0.2155530947	0.0931178515
C8	2.0554612969	1.1217881071	1.0104348396
O9	2.0799584816	-0.4615347317	-0.7606733736
C10	3.4847030771	1.1869567970	0.8900414267
C11	4.2614736600	2.0016697245	1.6953995940

C12	3.6867769338	2.8195575444	2.6860633262
C13	2.2831641394	2.7735895121	2.8233242443
C14	1.4915160743	1.9621992901	2.0235854870
H15	0.0672390022	-1.3650895340	-1.4995808341
H16	-3.8349552033	-0.6808461393	-0.1863722504
H17	-2.9451502145	0.9441178531	1.4904835351
H18	3.9125228096	0.5509119120	0.1230710190
H19	5.3456034454	2.0095292179	1.5565450943
H20	4.2980570859	3.4616383011	3.3179887807
H21	1.7998707351	3.3938957818	3.5813421715
H22	0.4170950388	1.9429454607	2.1471896171

#####mol75#####

#####mol#####

22

structure

C1	-0.0714118746	0.0349685102	-0.0737506068
C2	-0.6586357757	-1.1737256020	0.3191308068
N3	-1.9769794219	-1.3483775680	0.3729502610
C4	-2.7207398827	-0.2846907593	0.0511123564
N5	-2.2834770086	0.9232662489	-0.3066739270
C6	-0.9578417623	1.0729147928	-0.3687683906
C7	1.4234648105	0.1631022390	-0.0441937492
C8	2.1200021602	1.0910177376	-0.9884695727
O9	2.0551863369	-0.4963934205	0.7623679084
C10	3.3868202570	1.5661940946	-0.6212884786
C11	4.0985821120	2.3996424410	-1.4728324821
C12	3.5647792446	2.7500596773	-2.7139305992
C13	2.3179317643	2.2638967676	-3.0985845393
C14	1.5935770554	1.4433505453	-2.2379289620
H15	-0.0283775136	-2.0142259793	0.5919762074
H16	-3.7978118658	-0.4178736254	0.0908339750
H17	-0.5962717978	2.0597710850	-0.6409539683
H18	3.7925050665	1.2657688402	0.3367179927
H19	5.0712243698	2.7739277391	-1.1750254980
H20	4.1233129676	3.3964417896	-3.3814342542
H21	1.9094956849	2.5206696672	-4.0690561216
H22	0.6336406200	1.0553763967	-2.5552608866

#####mol\_reduced#####

22

structure

C1	-0.0752035647	0.0408133011	-0.1081756332
C2	-0.6413086016	-1.0715241601	0.5795224307
N3	-1.9450952949	-1.3066189338	0.6653119608
C4	-2.7520910770	-0.4039762569	0.0826682213
N5	-2.3639936818	0.7223771108	-0.5362968031
C6	-1.0518288153	0.9326154485	-0.6198269702
C7	1.3786815242	0.1915064694	-0.1036282371
C8	2.0833772900	1.1224810325	-1.0083177076
O9	2.0627406988	-0.5031143123	0.7100918373

C10	3.4235726287	1.4536876187	-0.6840287386
C11	4.1827911395	2.2904527365	-1.4856515577
C12	3.6545210132	2.8256572552	-2.6669066016
C13	2.3483567705	2.4808889587	-3.0275834224
C14	1.5798112106	1.6486797713	-2.2222149246
H15	0.0361349290	-1.7651146400	1.0657926495
H16	-3.8213291696	-0.5925060838	0.1352787109
H17	-0.7574371664	1.8702935152	-1.0800342181
H18	3.8285220791	1.0141889542	0.2190608800
H19	5.2019074988	2.5314002784	-1.1931055623
H20	4.2492590675	3.4803075636	-3.2959058497
H21	1.9276574865	2.8545188452	-3.9575332785
H22	0.5921922521	1.3670220273	-2.5635087362

#####mol\_double\_reduced#####

22

structure

C1	-0.0763460425	0.0692294974	-0.1208782452
C2	-0.6347387733	-0.9669849211	0.7286303051
N3	-1.9187268950	-1.2836445215	0.7954252742
C4	-2.7662419211	-0.5419055149	0.0423082925
N5	-2.4154073798	0.5421972628	-0.6913323910
C6	-1.1203177677	0.8331441839	-0.7536323204
C7	1.3554266270	0.2470461961	-0.0995598679
C8	2.0512709069	1.1456027519	-1.0024681255
O9	2.0550679163	-0.4319612528	0.7713707451
C10	3.4614249038	1.3505823502	-0.7578538221
C11	4.2446549239	2.1748693169	-1.5398166206
C12	3.7226231357	2.8570619171	-2.6612144443
C13	2.3629543113	2.6241120392	-2.9653625670
C14	1.5623162611	1.8072923439	-2.1837868647
H15	0.0704775980	-1.5100404472	1.3500079763
H16	-3.8253603611	-0.7963228138	0.0815650581
H17	-0.8847303817	1.7480763141	-1.2896296304
H18	3.8620341635	0.8065050461	0.0897928362
H19	5.3009455243	2.2968573595	-1.2854801043
H20	4.3420839690	3.5053907718	-3.2770287389
H21	1.9265796036	3.0814513513	-3.8561270943
H22	0.5494868857	1.6262643810	-2.5200351163

#####mol76#####

#####mol#####

22

structure

C1	-0.0707927917	0.0430137591	0.0687016183
C2	-0.6497311571	-1.1905782887	-0.2687395410
N3	-1.9594589574	-1.4034218775	-0.3420030409
N4	-2.8028774338	-0.3942477838	-0.1133482983
C5	-2.3158101259	0.8063534248	0.1908796322
C6	-0.9521290945	1.0852676812	0.3047133435
C7	1.4298275887	0.1730868749	0.0494858723

C8	2.1157822302	1.0962538001	1.0040103960
O9	2.0610380458	-0.4800780306	-0.7601636663
C10	3.3946557296	1.5580819757	0.6617851534
C11	4.0963856291	2.3864815990	1.5263457118
C12	3.5398684584	2.7449099723	2.7551887298
C13	2.2803234326	2.2721439343	3.1148639721
C14	1.5660204498	1.4566481543	2.2412416113
H15	-0.0189638403	-2.0447326767	-0.4868627511
H16	-3.0616974693	1.5780506368	0.3497786177
H17	-0.6110099537	2.0843149472	0.5468773810
H18	3.8173218238	1.2515248736	-0.2868931994
H19	5.0789336798	2.7500471841	1.2487159119
H20	4.0909743108	3.3867320074	3.4331180086
H21	1.8549858248	2.5347614528	4.0764454661
H22	0.5956118295	1.0786401385	2.5380867700

#####mol\_reduced#####

22

structure

C1	-0.0601221532	0.0357199804	0.1107805400
C2	-0.6376655352	-1.0777219531	-0.5769244402
N3	-1.9228993733	-1.3107294902	-0.7444347761
N4	-2.8436407624	-0.4325819776	-0.2596080142
C5	-2.3708775151	0.6617160354	0.3536848538
C6	-1.0341118484	0.9555426347	0.5701817757
C7	1.3887461251	0.1253606210	0.1758004137
C8	2.0784881720	1.1005152415	1.0643851854
O9	2.1052843763	-0.6255571067	-0.5496614147
C10	3.4159446657	1.4311218106	0.7507093986
C11	4.1561518084	2.2976171010	1.5412855096
C12	3.6022723433	2.8561854349	2.6976280916
C13	2.2949989562	2.5121118690	3.0474422339
C14	1.5467288667	1.6524196234	2.2491455827
H15	0.0386858998	-1.8101901533	-1.0046109328
H16	-3.1401064365	1.3552657005	0.6910303391
H17	-0.7658408417	1.8940690432	1.0374525741
H18	3.8410500304	0.9682573981	-0.1312852996
H19	5.1777675566	2.5399177874	1.2604355348
H20	4.1817424620	3.5311471106	3.3194591073
H21	1.8570700641	2.9069986809	3.9601579934
H22	0.5531150163	1.3714340298	2.5730751330

#####mol\_double\_reduced#####

22

structure

C1	-0.0560899896	0.0711278424	0.1183422024
C2	-0.6178380020	-0.9867129086	-0.7005290497
N3	-1.8819701914	-1.3069329905	-0.8531513245
N4	-2.8711291757	-0.5799184013	-0.2146288283
C5	-2.4261345146	0.4878451110	0.4843539939
C6	-1.1159479129	0.8706770422	0.6874722695



C7	1.3738714092	0.1942085955	0.1492806569
C8	2.0496236417	1.1281038079	1.0483355914
O9	2.1124889636	-0.5321591096	-0.6426714498
C10	3.4657973388	1.3027827196	0.8549906775
C11	4.2273153373	2.1489464921	1.6378745389
C12	3.6634677488	2.8773242443	2.7053976964
C13	2.2908219255	2.6771388368	2.9591272036
C14	1.5143477917	1.8400852392	2.1717541648
H15	0.1021495752	-1.5885899568	-1.2492863318
H16	-3.2272947743	1.0989637788	0.9155322493
H17	-0.9270911981	1.8020401490	1.2067952793
H18	3.8917039758	0.7174541973	0.0481466764
H19	5.2943852755	2.2512096430	1.4262920963
H20	4.2634475155	3.5446768424	3.3202350126
H21	1.8232651340	3.1768074221	3.8097265732
H22	0.4840152974	1.6831080147	2.4619136158

#####mol77#####

#####mol#####

23

structure

C1	3.6100042683	-2.6325249558	0.1094632169
C2	2.2196175679	-2.6101861904	0.1130165458
C3	1.5291891558	-1.3940350496	0.1067944528
C4	2.2667716149	-0.1918936531	0.0968375016
C5	3.6650366368	-0.2275246259	0.0933657534
C6	4.3380239198	-1.4414185633	0.0996365817
C7	0.0487610184	-1.3770969319	0.1106469473
C8	-0.6620341905	-0.1611784455	0.1044236117
C9	0.0385574805	1.1471575252	0.0938018535
C10	1.5915875983	1.1305043375	0.0898177104
N11	-0.5800417772	-2.5619260803	0.1202482631
C12	-1.9112353764	-2.5750179733	0.1239073872
C13	-2.7012447853	-1.4232906997	0.1183279568
C14	-2.0584285259	-0.1967454471	0.1083986431
O15	2.1890250339	2.1828249459	0.0812194164
O16	-0.5487847629	2.2047351065	0.0882507202
H17	4.1287392378	-3.5845595374	0.1143911571
H18	1.6459091093	-3.5270063462	0.1206306142
H19	4.1991099333	0.7146366376	0.0856899507
H20	5.4215347489	-1.4627391640	0.0968979599
H21	-2.3743672818	-3.5579733310	0.1317207616
H22	-3.7815699423	-1.4976025768	0.1217267293
H23	-2.6017836285	0.7406115673	0.1035839927

#####mol\_reduced#####

23

structure

C1	3.6217723873	-2.6354765597	0.1094856278
C2	2.2380004757	-2.6287252347	0.1131401047
C3	1.5169424588	-1.4199358127	0.1070111226

C4	2.2231954114	-0.1875263604	0.0969047333
C5	3.6333907545	-0.2217173394	0.0933432096
C6	4.3255704537	-1.4171032960	0.0994654948
C7	0.0618107940	-1.4049767118	0.1107968552
C8	-0.6178655200	-0.1542963973	0.1042682058
C9	0.0701099715	1.1474671608	0.0937579606
C10	1.5543745617	1.1322768772	0.0899055506
N11	-0.5955195676	-2.5851182291	0.1204186605
C12	-1.9214868646	-2.5753241133	0.1238900624
C13	-2.6879011202	-1.3977185614	0.1180792859
C14	-2.0243795011	-0.1874810458	0.1082383456
O15	2.2208564816	2.1855116438	0.0811060673
O16	-0.5828424586	2.2123175792	0.0883964100
H17	4.1604931552	-3.5784353689	0.1143378947
H18	1.6710511204	-3.5517098874	0.1208134370
H19	4.1427005575	0.7348999437	0.0855848861
H20	5.4120558385	-1.4170242427	0.0965456286
H21	-2.4091123603	-3.5492646610	0.1316829243
H22	-3.7722582248	-1.4510904217	0.1213303772
H23	-2.5423429219	0.7649459958	0.1032702997

#####mol\_double\_reduced#####

23

structure

C1	3.6373097799	-2.6444239422	0.1095016054
C2	2.2569025642	-2.6455568751	0.1132442511
C3	1.5015250047	-1.4491357148	0.1072911775
C4	2.1972727312	-0.1768028328	0.0969064529
C5	3.6214321999	-0.2197436112	0.0933228569
C6	4.3315526859	-1.3975878339	0.0992766001
C7	0.0769676108	-1.4376130369	0.1110071712
C8	-0.5937095033	-0.1444400125	0.1041639387
C9	0.0709653942	1.1495423003	0.0937691476
C10	1.5523842783	1.1336103291	0.0898944647
N11	-0.6147031904	-2.6097834930	0.1206436200
C12	-1.9363490769	-2.5825526217	0.1239397122
C13	-2.6939729551	-1.3779786818	0.1179209016
C14	-2.0102208432	-0.1834501270	0.1081682812
O15	2.2345475273	2.2030835827	0.0809173593
O16	-0.5951092096	2.2311713017	0.0883464167
H17	4.1896899560	-3.5834429876	0.1142876218
H18	1.6979252096	-3.5770222574	0.1209831501
H19	4.1128866210	0.7490826290	0.0854981958
H20	5.4221178197	-1.3818517586	0.0962103563
H21	-2.4449677870	-3.5512575513	0.1317148351
H22	-3.7831703174	-1.4162404812	0.1210479050
H23	-2.5085361913	0.7824183484	0.1030572341

#####mol78#####

#####mol#####

23

structure

C1	1.3567592210	-3.4977219158	0.1086779556
C2	1.3520312128	-2.1074237500	0.1132971711
C3	0.1508572779	-1.3841604801	0.1069982966
C4	-1.0573726088	-2.1181834694	0.0957614068
C5	-1.0409922553	-3.5173546054	0.0911915873
C6	0.1588071197	-4.2117583833	0.0975845047
C7	0.1295867575	0.0963727261	0.1118126748
C8	-1.0845931206	0.8088505683	0.1054282011
C9	-2.3977883381	0.1061585877	0.0935485013
C10	-2.3796083483	-1.4430467639	0.0884209239
C11	1.3015629305	0.8725066679	0.1228939112
N12	1.3291556494	2.2032674960	0.1275877003
C13	0.1602448152	2.8549656123	0.1213432679
C14	-1.0643348220	2.2028406146	0.1102825541
O15	-3.4314838376	-2.0415764093	0.0787179210
O16	-3.4533872207	0.6941560522	0.0878930334
H17	2.3037422959	-4.0253367950	0.1137882016
H18	2.3019087343	-1.5909104923	0.1219269087
H19	-1.9925845990	-4.0343617611	0.0825493584
H20	0.1650203139	-5.2951687552	0.0939994758
H21	2.2762064052	0.3981471879	0.1283294389
H22	0.2139462730	3.9392488650	0.1254017891
H23	-2.0006336768	2.7465186520	0.1053551392

#####mol\_reduced#####

23

structure

C1	1.3623103487	-3.5048635983	0.1086847241
C2	1.3703928114	-2.1205373040	0.1133896219
C3	0.1751173352	-1.3723074654	0.1072094647
C4	-1.0591934790	-2.0779634249	0.0958749120
C5	-1.0434146946	-3.4873182519	0.0912503588
C6	0.1404680898	-4.1975625644	0.0974727657
C7	0.1499670290	0.0865709636	0.1119270804
C8	-1.0995812178	0.7640642526	0.1051610655
C9	-2.3982908266	0.0771541760	0.0934561977
C10	-2.3805291114	-1.4066013804	0.0885486980
C11	1.3100822859	0.8835240273	0.1230088774
N12	1.3386074479	2.2131609279	0.1276927231
C13	0.1373485193	2.8371801536	0.1210891024
C14	-1.0687485532	2.1735796676	0.1101229804
O15	-3.4304038398	-2.0738850790	0.0786600964
O16	-3.4659189386	0.7249122329	0.0879413465
H17	2.3012485859	-4.0497631696	0.1136824456
H18	2.3249614639	-1.6079316503	0.1220562347
H19	-2.0081682441	-3.9808084128	0.0825760362
H20	0.1288752424	-5.2834032609	0.0937385354
H21	2.2874057578	0.4079075228	0.1284874598
H22	0.1713173151	3.9247486970	0.1249937415

H23 -2.0158348757 2.6994134322 0.1050446740  
#####mol\_double\_reduced#####

23

structure

C1	1.3756285638	-3.5150924220	0.1087032965
C2	1.3857157086	-2.1314082525	0.1134632957
C3	0.2013314468	-1.3576956576	0.1074782278
C4	-1.0696690205	-2.0530529408	0.0959007431
C5	-1.0413485590	-3.4762949569	0.0912867185
C6	0.1290162521	-4.1994734880	0.0973296197
C7	0.1731237057	0.0762386781	0.1120949905
C8	-1.1165771667	0.7385431064	0.1049455931
C9	-2.4050235192	0.0771180352	0.0934071900
C10	-2.3819345509	-1.4036416160	0.0885823943
C11	1.3202256526	0.8947399523	0.1231685613
N12	1.3585326742	2.2256485179	0.1278930855
C13	0.1249017363	2.8369247177	0.1209550099
C14	-1.0670045912	2.1637478097	0.1100500540
O15	-3.4458186863	-2.0904067278	0.0785640468
O16	-3.4913151919	0.7350379245	0.0877664782
H17	2.3128511492	-4.0694881017	0.1136272403
H18	2.3461776410	-1.6217666319	0.1221611219
H19	-2.0156412388	-3.9560879732	0.0825834789
H20	0.1045837078	-5.2894767078	0.0934442108
H21	2.3013046062	0.4158308553	0.1286962424
H22	0.1468532910	3.9291821445	0.1247384784
H23	-2.0219316004	2.6807690413	0.1048217921

#####mol79#####

#####mol#####

23

structure

C1	1.3486819661	-3.5313071970	0.1090070706
C2	1.3596791903	-2.1410572867	0.1134102939
C3	0.1670422269	-1.4056967099	0.1067582000
C4	-1.0505722990	-2.1219797602	0.0954151983
C5	-1.0513163212	-3.5202997721	0.0910368850
C6	0.1411136189	-4.2287089549	0.0977729985
C7	0.1654454320	0.0754466281	0.1113445844
C8	-1.0443488681	0.7990967784	0.1046308309
C9	-2.3628088433	0.1227562222	0.0927206290
C10	-2.3652350723	-1.4266824970	0.0877717183
C11	1.3393580820	0.8377693860	0.1224045210
C12	1.2607097429	2.2256110095	0.1261408866
N13	0.1141125069	2.9169313348	0.1198195840
C14	-1.0060113815	2.1992411074	0.1092912993
O15	-3.4214186558	-2.0165797786	0.0779807571
O16	-3.4155040052	0.7188969117	0.0868043931
H17	2.2884427606	-4.0714588524	0.1143819237
H18	2.3146004015	-1.6331308952	0.1221556191

H19	-2.0089824169	-4.0258610723	0.0822751112
H20	0.1336972645	-5.3121713849	0.0943380248
H21	2.3166664885	0.3752801360	0.1281974691
H22	2.1722265384	2.8167878584	0.1347184292
H23	-1.9452107255	2.7422688963	0.1040393990

#####mol\_reduced#####

23

structure

C1	1.3551770013	-3.5364859984	0.1090107672
C2	1.3775527751	-2.1540277803	0.1134730903
C3	0.1900803883	-1.3917966810	0.1069683119
C4	-1.0567789861	-2.0813974485	0.0955075931
C5	-1.0536077367	-3.4931137114	0.0911307931
C6	0.1216580724	-4.2144457354	0.0976755404
C7	0.1887010139	0.0615119058	0.1114840997
C8	-1.0498097641	0.7585234532	0.1044558828
C9	-2.3630296702	0.0901933938	0.0925906361
C10	-2.3645189236	-1.3972479851	0.0878858360
C11	1.3543352165	0.8545471178	0.1225998151
C12	1.2606549895	2.2318722117	0.1261868468
N13	0.0892545972	2.9094810525	0.1196152983
C14	-1.0110868753	2.1693088945	0.1091443793
O15	-3.4271685784	-2.0481333478	0.0778902589
O16	-3.4212781898	0.7459979426	0.0867819042
H17	2.2867777911	-4.0936954962	0.1142502394
H18	2.3366883705	-1.6486778992	0.1222164714
H19	-2.0232900337	-3.9768854193	0.0823714390
H20	0.0977497002	-5.3001773468	0.0941150677
H21	2.3379022834	0.3990936411	0.1284820226
H22	2.1621973585	2.8407342668	0.1347577562
H23	-1.9649510160	2.6877073586	0.1036809290

#####mol\_double\_reduced#####

23

structure

C1	1.3669112732	-3.5484250696	0.1090253069
C2	1.3955406273	-2.1709206514	0.1135310996
C3	0.2178566527	-1.3740590572	0.1072351858
C4	-1.0686448223	-2.0612272498	0.0955035159
C5	-1.0522099844	-3.4845134666	0.0911831690
C6	0.1069947458	-4.2229627503	0.0975279954
C7	0.2191561529	0.0432933584	0.1116609091
C8	-1.0577550592	0.7394566664	0.1043164210
C9	-2.3634122528	0.0884813842	0.0925665971
C10	-2.3657654082	-1.3997731216	0.0879015838
C11	1.3707923906	0.8741432431	0.1228213865
C12	1.2663099203	2.2447896096	0.1262961965
N13	0.0694735826	2.9247039678	0.1194895486
C14	-1.0108249431	2.1565424133	0.1090633662
O15	-3.4489452654	-2.0571723045	0.0777814697

O16	-3.4398805178	0.7517848706	0.0866077154
H17	2.2968424151	-4.1158464965	0.1141960524
H18	2.3626521126	-1.6717127760	0.1222978606
H19	-2.0319614078	-3.9541290244	0.0824150767
H20	0.0704808113	-5.3123304669	0.0938578930
H21	2.3645358713	0.4300454276	0.1288466371
H22	2.1639427653	2.8660752333	0.1349025044
H23	-1.9781452166	2.6563172024	0.1034148576

#####mol80#####

#####mol#####

23

structure

C1	1.3480210609	-3.5248369611	0.1119718550
C2	1.3649689983	-2.1346238488	0.1163586277
C3	0.1764312964	-1.3910249676	0.1067309156
C4	-1.0418737698	-2.1045837797	0.0923678524
C5	-1.0493992866	-3.5031582499	0.0880601620
C6	0.1383514267	-4.2184526990	0.0977778267
C7	0.1863190271	0.0918387205	0.1113575258
C8	-1.0129434244	0.8371987177	0.1015524106
C9	-2.3468441865	0.1482970361	0.0859580653
C10	-2.3512428687	-1.4024896665	0.0813563218
C11	1.3770223762	0.8348255522	0.1256314989
C12	1.3305524078	2.2182866202	0.1294419852
C13	0.0836053270	2.8472763803	0.1188311506
N14	-1.0593858759	2.1746261308	0.1052115930
O15	-3.4104550969	-1.9876366630	0.0690282621
O16	-3.3947294999	0.7412018444	0.0770236178
H17	2.2861989813	-4.0679995030	0.1196958174
H18	2.3244151242	-1.6354118215	0.1274629908
H19	-2.0102097728	-4.0028264909	0.0769324009
H20	0.1259817007	-5.3018757289	0.0943708146
H21	2.3393714702	0.3410245455	0.1337995662
H22	2.2416483161	2.8046367667	0.1404314402
H23	0.0072819475	3.9309218726	0.1214310150

#####mol\_reduced#####

23

structure

C1	1.3578288788	-3.5276174198	0.1120908421
C2	1.3840569433	-2.1437981642	0.1165576572
C3	0.2004015267	-1.3766575198	0.1070179898
C4	-1.0436657682	-2.0639796019	0.0924455132
C5	-1.0478112425	-3.4750481328	0.0881156809
C6	0.1242393521	-4.2024559058	0.0976665460
C7	0.2038402399	0.0819812841	0.1115051704
C8	-1.0346062300	0.8013236137	0.1012550244
C9	-2.3493333371	0.1193696031	0.0858919827
C10	-2.3465532750	-1.3704088686	0.0814688169
C11	1.3845132688	0.8403197812	0.1256907560

C12	1.3347006010	2.2228618123	0.1294487170
C13	0.0689196443	2.8292941269	0.1186123206
N14	-1.0668688151	2.1597019529	0.1051192154
O15	-3.4085918617	-2.0200744993	0.0688640709
O16	-3.4135377388	0.7565611603	0.0770066553
H17	2.2889198669	-4.0859246281	0.1197337171
H18	2.3476930362	-1.6473845021	0.1277359625
H19	-2.0205996896	-3.9523764690	0.0769023140
H20	0.0965319141	-5.2881521382	0.0940870539
H21	2.3490310271	0.3455878639	0.1338649582
H22	2.2390521362	2.8220179228	0.1403795084
H23	-0.0126600160	3.9169438411	0.1211638123

#####mol\_double\_reduced#####

23

structure

C1	1.3746802800	-3.5361743424	0.1122465126
C2	1.4005804725	-2.1535142440	0.1167258219
C3	0.2271159410	-1.3614468490	0.1073526195
C4	-1.0533627479	-2.0414968942	0.0924046829
C5	-1.0429291027	-3.4669781938	0.0881503077
C6	0.1157380628	-4.2058809248	0.0975479702
C7	0.2263133046	0.0699457369	0.1117099460
C8	-1.0549046513	0.7829466599	0.1010083745
C9	-2.3577560175	0.1203386463	0.0858532770
C10	-2.3455742983	-1.3705515228	0.0814549361
C11	1.3957724697	0.8480434377	0.1258218807
C12	1.3486037150	2.2314447340	0.1295780762
C13	0.0594566304	2.8310030838	0.1184859915
N14	-1.0667795685	2.1639747763	0.1051259418
O15	-3.4244986623	-2.0340062978	0.0685891764
O16	-3.4428757431	0.7563314158	0.0768309103
H17	2.3049953971	-4.1023362980	0.1198737462
H18	2.3699962306	-1.6593718081	0.1279744459
H19	-2.0241641565	-3.9325414946	0.0768482702
H20	0.0769589362	-5.2956092568	0.0938240939
H21	2.3646634311	0.3530509006	0.1340322309
H22	2.2520578277	2.8382284999	0.1404996519
H23	-0.0208232797	3.9259047270	0.1210462723

#####mol81#####

#####mol#####

22

structure

C1	1.3468246352	-3.3320544230	0.1066136774
N2	1.3196382680	-2.0012482646	0.1100405431
C3	0.1288541927	-1.3929294806	0.1034944260
C4	-1.0814195650	-2.1152497401	0.0931900032
C5	-1.0292363286	-3.5117616377	0.0897399953
C6	0.2052989480	-4.1377317551	0.0965477528
C7	0.1181971167	0.0982492349	0.1074603925

C8	-1.1022835227	0.8032034306	0.1009796774
C9	-2.4145587224	0.1099126250	0.0900927787
C10	-2.4034768121	-1.4407465579	0.0859180281
N11	1.3001507629	0.7235173126	0.1172704151
C12	1.3082851243	2.0545768927	0.1209099557
C13	0.1553388224	2.8438646372	0.1151120245
C14	-1.0700986186	2.2003216891	0.1049697654
O15	-3.4513501526	-2.0446393807	0.0770234322
O16	-3.4709537189	0.6988088994	0.0844599721
H17	2.3355285065	-3.7833383171	0.1122073983
H18	-1.9595450668	-4.0667441136	0.0818070855
H19	0.2931339024	-5.2172275187	0.0942132984
H20	2.2904269195	2.5199383370	0.1289213935
H21	0.2277072431	3.9245047936	0.1185233833
H22	-2.0082574184	2.7419639296	0.0999934204

#####mol\_reduced#####

22

structure

C1	1.3441074756	-3.3460861254	0.1065253733
N2	1.3455733898	-2.0220645944	0.1101513901
C3	0.1595924112	-1.3776288351	0.1037383384
C4	-1.0854889037	-2.0684771765	0.0932967191
C5	-1.0404591608	-3.4747117434	0.0897576234
C6	0.1749360769	-4.1262312412	0.0963319059
C7	0.1491345347	0.0833942842	0.1076275110
C8	-1.1057002355	0.7563954884	0.1007934583
C9	-2.4146363315	0.0749685253	0.0899717583
C10	-2.4040373293	-1.4058060448	0.0860548147
N11	1.3257701201	0.7446985880	0.1175382029
C12	1.3053673396	2.0685621585	0.1209683744
C13	0.1251507786	2.8319391111	0.1148617341
C14	-1.0807940582	2.1631299181	0.1047412116
O15	-3.4546182103	-2.0788600844	0.0770434925
O16	-3.4747444448	0.7329515560	0.0844693363
H17	2.3223552744	-3.8262726204	0.1119621744
H18	-1.9886458939	-4.0000056921	0.0818005181
H19	0.2387326369	-5.2101494971	0.0938046548
H20	2.2766447617	2.5626649343	0.1290185783
H21	0.1734348279	3.9166568663	0.1181108121
H22	-2.0364027436	2.6748310037	0.0995237136

#####mol\_double\_reduced#####

22

structure

C1	1.3478631938	-3.3636177909	0.1065252709
N2	1.3726372669	-2.0461348494	0.1102917858
C3	0.1948949788	-1.3592784490	0.1040458553
C4	-1.0944981906	-2.0420731386	0.0933126459
C5	-1.0466542769	-3.4576903854	0.0897617204
C6	0.1507111086	-4.1337874621	0.0961562485



C7	0.1846938811	0.0655396005	0.1078269583
C8	-1.1143484783	0.7298650561	0.1006759016
C9	-2.4160679107	0.0734940941	0.0899619925
C10	-2.4054877142	-1.4043340127	0.0860405599
N11	1.3524892050	0.7691336277	0.1177643765
C12	1.3088520317	2.0861193896	0.1210119628
C13	0.1007992065	2.8391364944	0.1147238753
C14	-1.0867742368	2.1460197915	0.1046833634
O15	-3.4726613405	-2.0911289214	0.0768412331
O16	-3.4929479214	0.7450051809	0.0843662150
H17	2.3195606887	-3.8688369065	0.1118435541
H18	-2.0107181796	-3.9592393270	0.0817406307
H19	0.1966987758	-5.2227429428	0.0934793164
H20	2.2732273278	2.6051473067	0.1290457869
H21	0.1312151957	3.9286362116	0.1178658488
H22	-2.0579133719	2.6337642235	0.0993136576

#####mol82#####

#####mol#####

22

structure

C1	1.3385294275	-3.3559799670	0.1085495682
N2	1.3082483174	-2.0248491798	0.1112103290
C3	0.1148078019	-1.4142831736	0.1041144770
C4	-1.0937123951	-2.1387859126	0.0940470816
C5	-1.0390289129	-3.5349640254	0.0914230585
C6	0.1964770941	-4.1603470404	0.0987678463
C7	0.1091369955	0.0629348803	0.1072181295
C8	-1.0936965692	0.7883772039	0.1002909061
C9	-2.4148580598	0.0984119975	0.0895239615
C10	-2.4113335422	-1.4557249275	0.0862203659
C11	1.3056633905	0.7949550351	0.1171963252
N12	1.3602782057	2.1264169674	0.1204118672
C13	0.2031468534	2.8001943660	0.1136897643
C14	-1.0410292169	2.1812528664	0.1036147113
O15	-3.4628922858	-2.0527531124	0.0775133132
O16	-3.4663283151	0.6922637218	0.0833932224
H17	2.3272514015	-3.8061713008	0.1145414973
H18	-1.9681780085	-4.0921142882	0.0836800835
H19	0.2850521421	-5.2395273646	0.0970586088
H20	2.2480228122	0.2607691097	0.1226963889
H21	0.2804713684	3.8832968543	0.1165325160
H22	-1.9614221835	2.7512933455	0.0983431757

#####mol\_reduced#####

22

structure

C1	1.3391055728	-3.3672737644	0.1085297545
N2	1.3345354488	-2.0415131986	0.1113543917
C3	0.1451929252	-1.4009734514	0.1043424898
C4	-1.0954121889	-2.0952962485	0.0941145354

C5	-1.0469987627	-3.4996777467	0.0914251302
C6	0.1721238557	-4.1481539203	0.0986086894
C7	0.1334573850	0.0522747256	0.1073630257
C8	-1.1061710210	0.7408158275	0.1000961991
C9	-2.4149147674	0.0649699589	0.0894529126
C10	-2.4101435770	-1.4204449477	0.0863130743
C11	1.3161903341	0.8128639136	0.1173154387
N12	1.3661821990	2.1420331070	0.1204957401
C13	0.1744172172	2.7854576383	0.1134505522
C14	-1.0481308751	2.1490045123	0.1034866514
O15	-3.4622644086	-2.0868878468	0.0774867090
O16	-3.4749619816	0.7221800524	0.0834013596
H17	2.3186663520	-3.8430658009	0.1144236101
H18	-1.9926997994	-4.0296827148	0.0836233605
H19	0.2392503722	-5.2314716434	0.0967446385
H20	2.2633057317	0.2827637511	0.1228662725
H21	0.2275973445	3.8727652119	0.1161259100
H22	-1.9819319264	2.6981450822	0.0980727502

#####mol\_double\_reduced#####

22

structure

C1	1.3474573898	-3.3813996326	0.1085821181
N2	1.3585885898	-2.0578313102	0.1115247682
C3	0.1776316903	-1.3860530945	0.1046245141
C4	-1.1032488479	-2.0694877427	0.0941150277
C5	-1.0494768665	-3.4846551203	0.0914189924
C6	0.1552098937	-4.1519947263	0.0984793428
C7	0.1595796604	0.0416419153	0.1075346658
C8	-1.1214440320	0.7125782244	0.0999458166
C9	-2.4197917824	0.0634077156	0.0894365150
C10	-2.4106176907	-1.4178599986	0.0863077298
C11	1.3267823427	0.8302473748	0.1174087204
N12	1.3813984003	2.1593581957	0.1205913766
C13	0.1552911560	2.7874767980	0.1132976147
C14	-1.0497803379	2.1365117290	0.1034604263
O15	-3.4761742319	-2.1036798343	0.0773092900
O16	-3.4973766783	0.7335284356	0.0833009688
H17	2.3222800326	-3.8768725732	0.1144021921
H18	-2.0084469622	-3.9953016149	0.0835303220
H19	0.2076817065	-5.2403504626	0.0964799805
H20	2.2789290719	0.3015589144	0.1229921997
H21	0.1934799562	3.8793675654	0.1158642119
H22	-1.9945519329	2.6719293153	0.0979547697

#####mol83#####

#####mol#####

22

structure

C1	1.3337283809	-3.3897529904	0.1053161121
N2	1.3192527099	-2.0582828561	0.1080185856

C3	0.1326940388	-1.4359557114	0.1029039198
C4	-1.0843641590	-2.1421158030	0.0948268402
C5	-1.0476364654	-3.5387149500	0.0921083915
C6	0.1806686317	-4.1785285862	0.0974300527
C7	0.1449793568	0.0439686644	0.1060894088
C8	-1.0539915295	0.7796203929	0.1011880971
C9	-2.3790850506	0.1153274133	0.0926128021
C10	-2.3947672147	-1.4389331864	0.0891952820
C11	1.3423225402	0.7595524194	0.1140278562
C12	1.2932262487	2.1498162958	0.1166921500
N13	0.1590686514	2.8636363626	0.1121174432
C14	-0.9821850073	2.1783411648	0.1045389155
O15	-3.4501114003	-2.0283444943	0.0821758319
O16	-3.4285177097	0.7159838747	0.0882137585
H17	2.3162926018	-3.8530215317	0.1096724979
H18	-1.9836642864	-4.0841926600	0.0859000833
H19	0.2557609808	-5.2588127939	0.0955919335
H20	2.2844147012	0.2289619107	0.1179718397
H21	2.2148639889	2.7248420396	0.1228450633
H22	-1.9050722158	2.7487581948	0.1007793526

#####mol\_reduced#####

22

structure

C1	1.3349472355	-3.3987072290	0.1052780534
N2	1.3450141586	-2.0747360743	0.1081379137
C3	0.1618463242	-1.4204078670	0.1031103671
C4	-1.0902425567	-2.0983669814	0.0949098995
C5	-1.0552919383	-3.5059104568	0.0921186394
C6	0.1551411784	-4.1661554593	0.0972592102
C7	0.1721133777	0.0293737822	0.1062052978
C8	-1.0570177947	0.7358700874	0.1010356667
C9	-2.3785995866	0.0781853730	0.0925319941
C10	-2.3922239420	-1.4110859358	0.0893220545
C11	1.3593025124	0.7830863617	0.1142063808
C12	1.2895690436	2.1617705293	0.1167023624
N13	0.1284480956	2.8592543296	0.1118805024
C14	-0.9900364695	2.1455161317	0.1043418779
O15	-3.4562736006	-2.0618374872	0.0821975676
O16	-3.4302749736	0.7422831356	0.0882621036
H17	2.3080715361	-3.8875733408	0.1095190247
H18	-2.0065258987	-4.0259341559	0.0858778143
H19	0.2100894410	-5.2502807516	0.0952589124
H20	2.3101835959	0.2649891106	0.1182794621
H21	2.2000041506	2.7576958718	0.1228662784
H22	-1.9308081984	2.6876276513	0.1003860588

#####mol\_double\_reduced#####

22

structure

C1	1.3415380932	-3.4143868218	0.1052927694
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N2	1.3744130336	-2.0986032577	0.1083270336
C3	0.1961698230	-1.4019256434	0.1034140987
C4	-1.0992312682	-2.0781365192	0.0949339282
C5	-1.0587635202	-3.4918201733	0.0921088128
C6	0.1354464319	-4.1765042845	0.0971016539
C7	0.2048210030	0.0094844513	0.1063961018
C8	-1.0635199146	0.7135348418	0.1009887857
C9	-2.3777938654	0.0759468266	0.0925278076
C10	-2.3930074829	-1.4134758872	0.0893122963
C11	1.3764694224	0.8089702424	0.1143493002
C12	1.2911632910	2.1788264771	0.1166951610
N13	0.1018028460	2.8765503039	0.1117389603
C14	-0.9930128321	2.1305847140	0.1043034291
O15	-3.4769233436	-2.0699902880	0.0820291942
O16	-3.4472168256	0.7490892141	0.0881201691
H17	2.3088386470	-3.9270545386	0.1094119104
H18	-2.0242101558	-3.9914739013	0.0857869787
H19	0.1756400138	-5.2649984115	0.0949553691
H20	2.3401221085	0.3076366654	0.1184998732
H21	2.1947961183	2.7911144524	0.1227913201
H22	-1.9503571393	2.6495564416	0.1002152402

#####mol84#####

#####mol#####

22

structure

C1	1.3340038607	-3.3803793240	0.1076483460
N2	1.3242553388	-2.0485431678	0.1103101678
C3	0.1399903371	-1.4200046913	0.1029950167
C4	-1.0776258356	-2.1239939429	0.0926892413
C5	-1.0462175580	-3.5202991013	0.0900710796
C6	0.1793227297	-4.1658787946	0.0976552717
C7	0.1640362287	0.0595722679	0.1062274005
C8	-1.0213744478	0.8188404198	0.0991224157
C9	-2.3634529204	0.1433612236	0.0878577385
C10	-2.3818546926	-1.4129113702	0.0846151857
C11	1.3793485736	0.7543829814	0.1165586433
C12	1.3624788078	2.1389184976	0.1193311979
C13	0.1277572592	2.7953996586	0.1116791913
N14	-1.0369330604	2.1567387430	0.1017978316
O15	-3.4406202534	-1.9967900935	0.0757147005
O16	-3.4077970322	0.7411343857	0.0813132147
H17	2.3153583677	-3.8464646477	0.1138163312
H18	-1.9850931019	-4.0609441847	0.0821432955
H19	0.2506354167	-5.2463779442	0.0959643742
H20	2.3029726644	0.1910353516	0.1221405546
H21	2.2844821332	2.7080333632	0.1272658646
H22	0.0789477141	3.8806844894	0.1136051515

#####mol\_reduced#####

22

structure

C1	1.3393451149	-3.3856736578	0.1076771398
N2	1.3505770765	-2.0598020681	0.1105187978
C3	0.1692743655	-1.4043424310	0.1032666766
C4	-1.0799532431	-2.0802272767	0.0927631699
C5	-1.0497767994	-3.4871517668	0.0900745913
C6	0.1599034460	-4.1508574830	0.0974954233
C7	0.1847831742	0.0490401111	0.1063750926
C8	-1.0404099763	0.7798745570	0.0988898668
C9	-2.3657239431	0.1095415478	0.0877977026
C10	-2.3757603548	-1.3822493000	0.0847334123
C11	1.3890335754	0.7658591780	0.1166787152
C12	1.3637368816	2.1481718033	0.1193459349
C13	0.1081913881	2.7790199866	0.1114361664
N14	-1.0461356310	2.1377707758	0.1016326730
O15	-3.4405380475	-2.0304788354	0.0756553019
O16	-3.4223949188	0.7564902055	0.0813129175
H17	2.3124659398	-3.8745279564	0.1137486068
H18	-2.0031205653	-4.0032725761	0.0820689309
H19	0.2129329263	-5.2351191353	0.0956277679
H20	2.3160088365	0.2050173349	0.1223232788
H21	2.2774654288	2.7335286177	0.1272580522
H22	0.0498704480	3.8683412880	0.1132621317

#####mol\_double\_reduced#####

22

structure

C1	1.3512109529	-3.3964869103	0.1077480267
N2	1.3753692500	-2.0737764854	0.1107116902
C3	0.2013451324	-1.3882345336	0.1035656495
C4	-1.0871771462	-2.0568737374	0.0927456655
C5	-1.0490205866	-3.4745760361	0.0900505842
C6	0.1463635357	-4.1554291912	0.0973495880
C7	0.2093368798	0.0373466832	0.1065787793
C8	-1.0596162495	0.7587339080	0.0987349599
C9	-2.3724538757	0.1083731319	0.0877669760
C10	-2.3741187806	-1.3832518110	0.0847396485
C11	1.4009090937	0.7790324620	0.1168136035
C12	1.3740255999	2.1608003210	0.1194121098
C13	0.0932611741	2.7819304880	0.1112793865
N14	-1.0486218677	2.1396389910	0.1016080869
O15	-3.4551080334	-2.0454658844	0.0754988375
O16	-3.4495401483	0.7567440884	0.0811591952
H17	2.3204002093	-3.9032725635	0.1137531565
H18	-2.0140954156	-3.9739639855	0.0819444945
H19	0.1864507046	-5.2444594383	0.0953468270
H20	2.3326420523	0.2203406391	0.1225030063
H21	2.2842105567	2.7577591288	0.1272799039
H22	0.0340015765	3.8781122032	0.1130561246

#####mol85#####

#####mol#####

22

structure

N1	1.3543163502	-3.5003497206	0.1085269866
C2	1.3274631889	-2.1694291670	0.1104067559
C3	0.1553306399	-1.3948881185	0.1032362943
C4	-1.0596950988	-2.1042162850	0.0934195373
C5	-1.0400711418	-3.4975759878	0.0913898938
C6	0.1849540089	-4.1505151212	0.0991451948
C7	0.1799770592	0.0844017700	0.1057589113
C8	-1.0158778679	0.8356253382	0.0983273814
C9	-2.3553756060	0.1561747395	0.0875353492
C10	-2.3712559203	-1.3957602507	0.0851006762
C11	1.3771534292	0.8170297276	0.1155616915
C12	1.3379784649	2.2007284090	0.1175057630
C13	0.0945094382	2.8374027971	0.1095741768
N14	-1.0534390105	2.1729388546	0.1002103771
O15	-3.4263608797	-1.9834584922	0.0766524086
O16	-3.4004793531	0.7530387749	0.0807841982
H17	2.3026242345	-1.6953907318	0.1181161638
H18	-1.9765380670	-4.0409182319	0.0838324544
H19	0.2375630038	-5.2348129200	0.0978332926
H20	2.3355176580	0.3155827375	0.1216707694
H21	2.2523328605	2.7818564278	0.1250322760
H22	0.0253974801	3.9214010003	0.1108362018

#####mol\_reduced#####

22

structure

N1	1.3699489767	-3.5048585873	0.1086455189
C2	1.3391370674	-2.1752716623	0.1104897805
C3	0.1766815011	-1.3821600739	0.1033992984
C4	-1.0708951783	-2.0601288686	0.0933879429
C5	-1.0383526647	-3.4697628556	0.0914485649
C6	0.1691428259	-4.1312217179	0.0990768233
C7	0.1989003653	0.0741499556	0.1058652362
C8	-1.0325715957	0.8000104604	0.0981421730
C9	-2.3575092570	0.1230724417	0.0874892318
C10	-2.3664612814	-1.3680815132	0.0851438120
C11	1.3868033989	0.8224248092	0.1156285954
C12	1.3429566456	2.2049592804	0.1175498777
C13	0.0820804060	2.8198344656	0.1094564989
N14	-1.0587462629	2.1558556116	0.1001404091
O15	-3.4324232411	-2.0136350054	0.0764907675
O16	-3.4123854255	0.7689164741	0.0808214269
H17	2.3163508984	-1.6981278931	0.1182317849
H18	-1.9841245096	-3.9979526519	0.0838605437
H19	0.2045398933	-5.2189255049	0.0976504281
H20	2.3475354646	0.3206602792	0.1217472605
H21	2.2510072836	2.7987154264	0.1250594363

H22 0.0068171443 3.9077464879 0.1106877614  
#####mol\_double\_reduced#####

22

structure

N1	1.3937083517	-3.5146273211	0.1088116283
C2	1.3502220217	-2.1830262514	0.1106070640
C3	0.1995399388	-1.3717613380	0.1036112992
C4	-1.0842372978	-2.0350817171	0.0933206622
C5	-1.0326404154	-3.4610918869	0.0914398247
C6	0.1615695413	-4.1294768403	0.0989761387
C7	0.2201106175	0.0634154239	0.1060286137
C8	-1.0509954644	0.7795980830	0.0979907856
C9	-2.3637713120	0.1216686039	0.0874817816
C10	-2.3685030618	-1.3685794110	0.0851314823
C11	1.3967584327	0.8274494324	0.1157168493
C12	1.3562764757	2.2127829460	0.1176119718
C13	0.0742610071	2.8184420202	0.1093350583
N14	-1.0585786350	2.1591373579	0.1001234718
O15	-3.4514464393	-2.0266100969	0.0763183956
O16	-3.4366609872	0.7729852891	0.0807411100
H17	2.3298663601	-1.7012931135	0.1184163376
H18	-1.9854058787	-3.9817881240	0.0837598986
H19	0.1873025120	-5.2215283748	0.0974342455
H20	2.3602370096	0.3238642211	0.1218657513
H21	2.2628070964	2.8143965075	0.1250926124
H22	0.0005846432	3.9133131140	0.1105379001

#####mol86#####

#####mol#####

22

structure

C1	1.3022040005	-3.4924400738	0.1068062954
C2	1.3569928322	-2.1030558913	0.1134724851
C3	0.1681974397	-1.3650130038	0.1036263020
C4	-1.0305279220	-2.1076186076	0.0871929987
C5	-0.9661910636	-3.5070060088	0.0818088457
N6	0.1675765044	-4.2027527138	0.0912349601
C7	0.1386189230	0.1126596379	0.1097939167
C8	-1.0833368085	0.8111260845	0.0993512329
C9	-2.3924004521	0.0949471199	0.0817253582
C10	-2.3612656514	-1.4552405099	0.0753806656
C11	1.3062649075	0.8921885989	0.1261473546
N12	1.3236119835	2.2232379334	0.1322067438
C13	0.1491351020	2.8642323645	0.1220236571
C14	-1.0727106140	2.2043800195	0.1055939168
O15	-3.4047095827	-2.0665390057	0.0612530939
O16	-3.4510499432	0.6755918300	0.0724695402
H17	2.2235113074	-4.0679400459	0.1144240507
H18	2.3249221114	-1.6214496824	0.1262213793
H19	-1.8943943294	-4.0684998164	0.0691702617

H20	2.2828873510	0.4212275399	0.1348802235
H21	0.1941890165	3.9488978456	0.1272953447
H22	-2.0118391337	2.7430240512	0.0975692968

#####mol\_reduced#####

22

structure

C1	1.3026885405	-3.4984964047	0.1068198769
C2	1.3741518664	-2.1194886088	0.1136596371
C3	0.1928052763	-1.3508633206	0.1039833779
C4	-1.0316041244	-2.0678127079	0.0873256844
C5	-0.9699955070	-3.4762662557	0.0818178061
N6	0.1448673540	-4.1958423854	0.0909659499
C7	0.1590499311	0.1012225629	0.1099712950
C8	-1.0977984427	0.7669152566	0.0990201647
C9	-2.3903435428	0.0691854080	0.0817291615
C10	-2.3608677343	-1.4191582678	0.0755104673
C11	1.3161006916	0.9034444755	0.1262605748
N12	1.3346018043	2.2310597280	0.1322818991
C13	0.1267665289	2.8468182119	0.1216306231
C14	-1.0752797724	2.1772380101	0.1054304215
O15	-3.4027104450	-2.0943203238	0.0610468373
O16	-3.4629364557	0.7054516949	0.0727195093
H17	2.2145071237	-4.0916275191	0.1142866762
H18	2.3483338493	-1.6453509116	0.1264985984
H19	-1.9135897860	-4.0126818017	0.0690364824
H20	2.2948707661	0.4299668947	0.1349998556
H21	0.1542559537	3.9342831620	0.1266973471
H22	-2.0248058079	2.6985151880	0.0972305924

#####mol\_double\_reduced#####

22

structure

C1	1.3101742912	-3.5094011869	0.1068279510
C2	1.3903992342	-2.1354605639	0.1137325398
C3	0.2222962681	-1.3327926758	0.1043856695
C4	-1.0382717306	-2.0465067360	0.0873594495
C5	-0.9680234112	-3.4625462358	0.0819338131
N6	0.1285939352	-4.2079193812	0.0907516558
C7	0.1828107447	0.0888049423	0.1101911394
C8	-1.1144320010	0.7441966102	0.0987244317
C9	-2.3959848127	0.0719249346	0.0816541531
C10	-2.3603434531	-1.4155535575	0.0755335601
C11	1.3277131325	0.9178970542	0.1264883969
N12	1.3541029497	2.2434368835	0.1325889289
C13	0.1134603222	2.8501752340	0.1215107476
C14	-1.0730211501	2.1685123428	0.1054043629
O15	-3.4169771109	-2.1054573554	0.0608560104
O16	-3.4900968794	0.7124196420	0.0723929890
H17	2.2185733621	-4.1141140972	0.1141796360
H18	2.3736982409	-1.6708111557	0.1265979542



H19	-1.9247493159	-3.9812886003	0.0691119228
H20	2.3107769122	0.4417327960	0.1352803003
H21	0.1303572824	3.9417285430	0.1264677096
H22	-2.0309368487	2.6803184798	0.0970434141

#####mol87#####

#####mol#####

22

structure

N1	1.3674799258	-3.4698619026	0.1095792704
C2	1.3188259047	-2.1397821979	0.1113509602
C3	0.1321677283	-1.3865996222	0.1043479540
C4	-1.0715340892	-2.1179498937	0.0948573066
C5	-1.0266265333	-3.5113580877	0.0929533695
C6	0.2101701345	-4.1413368091	0.1005063561
C7	0.1232657321	0.0908180720	0.1066473948
C8	-1.0891741658	0.8076220849	0.0994452207
C9	-2.4066442145	0.1120727760	0.0892206843
C10	-2.3972917064	-1.4383058933	0.0867580909
C11	1.3007471573	0.8582339713	0.1159881226
N12	1.3333376632	2.1888091535	0.1183662628
C13	0.1680096040	2.8462972586	0.1114014819
C14	-1.0610903391	2.2014734242	0.1018882541
O15	-3.4441125597	-2.0407277997	0.0785022138
O16	-3.4606577414	0.7018497555	0.0828868180
H17	2.2844598714	-1.6473923390	0.1188024598
H18	-1.9524776971	-4.0725332804	0.0856565747
H19	0.2825697273	-5.2244183013	0.0992860485
H20	2.2722515478	0.3775145582	0.1218929651
H21	0.2273246772	3.9301742070	0.1135638001
H22	-1.9936463354	2.7514538195	0.0963509861

#####mol\_reduced#####

22

structure

N1	1.3777128938	-3.4796238199	0.1096056642
C2	1.3298427066	-2.1507396489	0.1113748812
C3	0.1543182998	-1.3761444902	0.1044992513
C4	-1.0822002403	-2.0739213124	0.0948531565
C5	-1.0296758622	-3.4810270411	0.0929868410
C6	0.1889602404	-4.1241579279	0.1003838396
C7	0.1455180466	0.0806491916	0.1067774028
C8	-1.0993382761	0.7634776804	0.0992767093
C9	-2.4063312938	0.0792707950	0.0891456123
C10	-2.3973652954	-1.4055144064	0.0868258289
C11	1.3116172759	0.8693242325	0.1161138666
N12	1.3434529607	2.1986935721	0.1184927341
C13	0.1470157150	2.8288609602	0.1112368580
C14	-1.0637849545	2.1711119097	0.1017971738
O15	-3.4493553158	-2.0718217615	0.0784853544
O16	-3.4662828789	0.7328633394	0.0828755205

H17	2.2982805342	-1.6575933761	0.1188303354
H18	-1.9670872983	-4.0238597702	0.0856533802
H19	0.2413102304	-5.2110647349	0.0990320799
H20	2.2859334510	0.3878916622	0.1220705282
H21	0.1862511417	3.9163214443	0.1132732536
H22	-2.0076741620	2.7026191566	0.0961327233

#####mol\_double\_reduced#####

22

structure

N1	1.3969709719	-3.4921347563	0.1097004643
C2	1.3398321589	-2.1607853252	0.1114406461
C3	0.1774780261	-1.3660786861	0.1046800246
C4	-1.0966881491	-2.0468827566	0.0947924030
C5	-1.0275258343	-3.4697100772	0.0929965446
C6	0.1772350603	-4.1221198730	0.1002722334
C7	0.1688172807	0.0708541776	0.1069248297
C8	-1.1134744245	0.7362658977	0.0991227138
C9	-2.4106580665	0.0772693291	0.0891211482
C10	-2.4017230043	-1.4035704669	0.0868236933
C11	1.3214925456	0.8795074978	0.1162129489
N12	1.3625652174	2.2114503794	0.1186419966
C13	0.1353228553	2.8266884447	0.1111265338
C14	-1.0614891326	2.1598223711	0.1017679390
O15	-3.4687334759	-2.0863631914	0.0783876219
O16	-3.4858377553	0.7471505250	0.0827732719
H17	2.3113188342	-1.6649585630	0.1189504207
H18	-1.9734968680	-4.0023323114	0.0856101685
H19	0.2172041705	-5.2136870035	0.0988040151
H20	2.2988893658	0.3954165327	0.1222099185
H21	0.1621110893	3.9186612792	0.1130644315
H22	-2.0138277505	2.6809927649	0.0960142061

#####mol88#####

#####mol#####

22

structure

C1	1.2908865126	-3.5274889356	0.1031882450
C2	1.3623790330	-2.1384008355	0.1098328167
C3	0.1825115525	-1.3886708270	0.1022119842
C4	-1.0258129662	-2.1127626659	0.0879596887
C5	-0.9793520652	-3.5125026119	0.0823545340
N6	0.1467166671	-4.2214890012	0.0896660939
C7	0.1733007649	0.0915241431	0.1085205502
C8	-1.0439503021	0.8006006000	0.1004068518
C9	-2.3586214755	0.1110793504	0.0853114597
C10	-2.3489667784	-1.4395626826	0.0786475552
C11	1.3437408708	0.8557934662	0.1225597650
C12	1.2549584887	2.2438912647	0.1277534799
N13	0.1022271073	2.9236715307	0.1201421785
C14	-1.0149258182	2.2008095202	0.1067551935

O15	-3.3971113956	-2.0418845656	0.0663079969
O16	-3.4141840354	0.7003919442	0.0781485603
H17	2.2041062755	-4.1156340412	0.1090580003
H18	2.3351512040	-1.6658760205	0.1208210967
H19	-1.9141442677	-4.0627830300	0.0713728119
H20	2.3223114075	0.3953212384	0.1295455248
H21	2.1607827800	2.8432945229	0.1386438735
H22	-1.9564907800	2.7394927858	0.1004509750

#####mol\_reduced#####

22

structure

C1	1.2922001784	-3.5318786524	0.1031834506
C2	1.3789146011	-2.1556326997	0.1099160629
C3	0.2061211232	-1.3720130741	0.1024853151
C4	-1.0308699068	-2.0731804441	0.0880607140
C5	-0.9827505435	-3.4845465205	0.0824235838
N6	0.1221198965	-4.2156439240	0.0894509318
C7	0.1971095381	0.0751534808	0.1086551656
C8	-1.0485216692	0.7609631883	0.1001820857
C9	-2.3560016617	0.0826402200	0.0852164578
C10	-2.3466962960	-1.4110816048	0.0787994764
C11	1.3600561771	0.8732244730	0.1227838481
C12	1.2562170499	2.2482942437	0.1277895948
N13	0.0777075709	2.9175221302	0.1198750474
C14	-1.0179774244	2.1728134486	0.1065865038
O15	-3.4020484030	-2.0675976994	0.0662116505
O16	-3.4194508723	0.7260408245	0.0782358532
H17	2.1954005883	-4.1377571773	0.1088916484
H18	2.3578334477	-1.6898856709	0.1209489342
H19	-1.9325476546	-4.0102741120	0.0714089802
H20	2.3446985388	0.4196087575	0.1298633951
H21	2.1517964216	2.8653091594	0.1386803471
H22	-1.9742472886	2.6867489327	0.1000362525

#####mol\_double\_reduced#####

22

structure

C1	1.2969812720	-3.5455058324	0.1031301944
C2	1.3968234270	-2.1783814829	0.1099726313
C3	0.2366487636	-1.3510590179	0.1028557145
C4	-1.0381896206	-2.0579707323	0.0880628810
C5	-0.9820934502	-3.4733705103	0.0824282883
N6	0.1023016751	-4.2354841704	0.0891103819
C7	0.2279045765	0.0545415138	0.1088587993
C8	-1.0556281185	0.7456514811	0.1000266055
C9	-2.3545879877	0.0841776576	0.0852521111
C10	-2.3452822800	-1.4125897009	0.0788677749
C11	1.3776741861	0.8961759568	0.1230915383
C12	1.2608047947	2.2619690024	0.1278979858
N13	0.0576290181	2.9371122430	0.1197021052

C14	-1.0171833900	2.1616311735	0.1064649615
O15	-3.4216933563	-2.0708838835	0.0661637064
O16	-3.4390872502	0.7291488530	0.0780984320
H17	2.1968004851	-4.1635681493	0.1087654892
H18	2.3869117144	-1.7258297262	0.1210769000
H19	-1.9458830017	-3.9803053517	0.0713467564
H20	2.3733322906	0.4559333183	0.1303797573
H21	2.1528544658	2.8911239188	0.1388294874
H22	-1.9872199354	2.6565852227	0.0996580356

#####mol89#####

#####mol#####

22

structure

C1	1.3585343041	-3.5203396226	0.1028777602
C2	1.3985954983	-2.1364636201	0.1096485738
C3	0.2024676143	-1.4047218756	0.1015705785
C4	-0.9953535240	-2.1511550272	0.0866410578
N5	-1.0345074192	-3.4877617544	0.0800899867
C6	0.1135617016	-4.1534553663	0.0880280419
C7	0.1818243500	0.0754132274	0.1081982701
C8	-1.0360589793	0.7825738437	0.0999901735
C9	-2.3456874940	0.0865503844	0.0843554717
C10	-2.3344806683	-1.4654873182	0.0769329427
C11	1.3484398420	0.8478184889	0.1227353297
C12	1.2543413610	2.2351526215	0.1282608576
N13	0.0998064997	2.9120996227	0.1205683880
C14	-1.0130541948	2.1827271975	0.1067211583
O15	-3.3777656099	-2.0645743795	0.0638438369
O16	-3.4040011261	0.6715113508	0.0772298906
H17	2.2713155080	-4.1037159273	0.1089287539
H18	2.3565430240	-1.6335412024	0.1211515755
H19	0.0424936872	-5.2373374864	0.0823469620
H20	2.3308100970	0.3955644984	0.1298762226
H21	2.1586936941	2.8370199013	0.1395187811
H22	-1.9578624626	2.7157643742	0.1003145851

#####mol\_reduced#####

22

structure

C1	1.3639187564	-3.5229701117	0.1028680449
C2	1.4076571896	-2.1424029708	0.1096504050
C3	0.2200367533	-1.3927098242	0.1017588791
C4	-1.0168472601	-2.1156504784	0.0866077438
N5	-1.0408753267	-3.4746863051	0.0800995598
C6	0.0984644526	-4.1361667749	0.0879443922
C7	0.2066871048	0.0586703675	0.1083361836
C8	-1.0364079587	0.7426288369	0.0997418829
C9	-2.3391848762	0.0552936400	0.0841872304
C10	-2.3345436908	-1.4397977901	0.0771466892
C11	1.3663939542	0.8607428021	0.1230076817

C12	1.2593465388	2.2368119919	0.1283817736
N13	0.0811967112	2.9036102694	0.1203584654
C14	-1.0119792252	2.1536622755	0.1065413661
O15	-3.3956364645	-2.0788393449	0.0639366345
O16	-3.4019710671	0.6985874121	0.0771636149
H17	2.2698333272	-4.1194855139	0.1087778467
H18	2.3674611388	-1.6379430542	0.1211640951
H19	0.0241453619	-5.2241094113	0.0822164157
H20	2.3546875978	0.4152470858	0.1302703434
H21	2.1548194123	2.8543574925	0.1396955646
H22	-1.9707457014	2.6627468771	0.0998504945

#####mol\_double\_reduced#####

22

structure

C1	1.3768852636	-3.5321637761	0.1029026383
C2	1.4218419167	-2.1550199686	0.1097139311
C3	0.2440479666	-1.3774331127	0.1020811830
C4	-1.0365585647	-2.1010617350	0.0865057126
N5	-1.0406880695	-3.4782108078	0.0800966836
C6	0.0870838552	-4.1423665971	0.0877874504
C7	0.2373784202	0.0393404545	0.1085651642
C8	-1.0417209978	0.7243055204	0.0995877157
C9	-2.3363244766	0.0552255152	0.0842225042
C10	-2.3415089158	-1.4434500294	0.0770864559
C11	1.3840332407	0.8768295222	0.1233012245
C12	1.2692633287	2.2465105592	0.1285302985
N13	0.0664898877	2.9179299605	0.1202262837
C14	-1.0073271551	2.1418904793	0.1064587074
O15	-3.4262780344	-2.0758815533	0.0636982073
O16	-3.4167589048	0.7070738780	0.0770836534
H17	2.2818985838	-4.1370067045	0.1087164946
H18	2.3875074873	-1.6528436497	0.1212536681
H19	0.0129908078	-5.2367883981	0.0820178033
H20	2.3815758847	0.4410139952	0.1307410833
H21	2.1617529914	2.8746861173	0.1398699152
H22	-1.9785597769	2.6338165534	0.0995100148

#####mol90#####

#####mol#####

22

structure

C1	1.3545642627	-3.5155315180	0.1048322371
C2	1.4016990874	-2.1319220489	0.1113263588
C3	0.2105595400	-1.3905649471	0.1010749616
C4	-0.9893204093	-2.1329308608	0.0843075013
N5	-1.0361663124	-3.4696347612	0.0780287662
C6	0.1069580633	-4.1429061163	0.0880597292
C7	0.2039028378	0.0909617778	0.1074124390
C8	-1.0026249225	0.8226103209	0.0970262634
C9	-2.3284260611	0.1157230836	0.0789217307

C10	-2.3214343441	-1.4378773408	0.0721690924
C11	1.3883220272	0.8428961105	0.1239810293
C12	1.3287200797	2.2260318385	0.1293774890
C13	0.0754942977	2.8422659874	0.1180374494
N14	-1.0615239917	2.1588451869	0.1022362961
O15	-3.3687129059	-2.0306226262	0.0575695365
O16	-3.3810013088	0.6991197855	0.0695265868
H17	2.2649544984	-4.1028127260	0.1125689670
H18	2.3645218353	-1.6385038831	0.1243263944
H19	0.0298339208	-5.2263905881	0.0825432917
H20	2.3555340682	0.3580469768	0.1327043463
H21	2.2337760783	2.8214176771	0.1421342146
H22	-0.0113838504	3.9250189207	0.1218469921

#####mol\_reduced#####

22

structure

C1	1.3635594938	-3.5154045050	0.1048960876
C2	1.4119751103	-2.1331208185	0.1114136313
C3	0.2289042321	-1.3783049960	0.1013426940
C4	-1.0061400217	-2.0974371041	0.0842843516
N5	-1.0384475261	-3.4557996824	0.0780560191
C6	0.0980358646	-4.1236900190	0.0880101298
C7	0.2223612559	0.0788469732	0.1075917130
C8	-1.0190928100	0.7869471470	0.0966600935
C9	-2.3244477523	0.0877149818	0.0787998406
C10	-2.3177210909	-1.4098381985	0.0723916374
C11	1.3985882741	0.8442084048	0.1241641786
C12	1.3377193883	2.2260072017	0.1295057983
C13	0.0667620081	2.8229789878	0.1178148846
N14	-1.0636321132	2.1449621792	0.1020957404
O15	-3.3790359334	-2.0461740076	0.0575751981
O16	-3.3914373473	0.7145903078	0.0693563678
H17	2.2683974982	-4.1137644969	0.1125004405
H18	2.3765528813	-1.6381633004	0.1244263553
H19	0.0185232934	-5.2113580511	0.0824327533
H20	2.3675915580	0.3578815602	0.1329509552
H21	2.2371154076	2.8324303452	0.1422692571
H22	-0.0225797848	3.9098924744	0.1215777445

#####mol\_double\_reduced#####

22

structure

C1	1.3814855934	-3.5207548528	0.1050585225
C2	1.4228876702	-2.1351494168	0.1115612489
C3	0.2496951756	-1.3669538045	0.1016545012
C4	-1.0235761675	-2.0792462095	0.0841627045
N5	-1.0349040390	-3.4625907446	0.0780182441
C6	0.0944358092	-4.1235032963	0.0879043875
C7	0.2432503428	0.0676866820	0.1078068637
C8	-1.0363667240	0.7686096467	0.0963735830

C9	-2.3282584444	0.0890608920	0.0787867760
C10	-2.3215209180	-1.4112263085	0.0723674929
C11	1.4094746086	0.8463238491	0.1243336475
C12	1.3555907988	2.2315076727	0.1297245938
C13	0.0631612089	2.8227531849	0.1177026122
N14	-1.0601723246	2.1517928745	0.1021023115
O15	-3.4027844317	-2.0490878634	0.0573457257
O16	-3.4152031442	0.7173024859	0.0691541964
H17	2.2866356352	-4.1244265753	0.1126418654
H18	2.3899793665	-1.6369820665	0.1246499973
H19	0.0191162554	-5.2187697878	0.0822851621
H20	2.3810227357	0.3568197110	0.1331713634
H21	2.2552551319	2.8432405964	0.1425160973
H22	-0.0220521725	3.9173055731	0.1214867068

#####mol91#####

#####mol#####

22

structure

C1	1.7096238849	-2.6486459184	1.3842483663
C2	2.6826716426	-1.7085904429	1.0480007368
C3	2.3224634174	-0.5007241240	0.4577728611
C4	0.9792358935	-0.2113577330	0.1929946171
C5	-0.0061364640	-1.1667492694	0.5350487611
C6	0.3713437985	-2.3722859601	1.1258959080
C7	0.5234283935	1.0236722819	-0.4188246747
C8	-0.8023708286	1.3492266957	-0.6981762072
C9	-1.8912961239	0.4380856813	-0.3867023882
C10	-1.4610392992	-0.9150605388	0.2766118005
C11	-0.8191464182	2.6431277540	-1.2938556428
C12	0.4826136309	3.0663778885	-1.3607104742
N13	1.2890390091	2.0774607742	-0.8276808742
O14	-2.3111806090	-1.7253066555	0.5650168203
O15	-3.0654966160	0.6506593441	-0.5994264940
H16	1.9939854368	-3.5877176133	1.8435384046
H17	3.7282206396	-1.9156402931	1.2457776331
H18	3.0993776496	0.2133589205	0.2061802976
H19	-0.4090079218	-3.0811135884	1.3748750113
H20	-1.6918031800	3.1807840627	-1.6262352551
H21	0.9089120065	3.9810511779	-1.7389184360
H22	2.2916361828	2.1349850668	-0.7561814330

#####mol\_reduced#####

22

structure

C1	1.6814054972	-2.6449329201	1.3799431152
C2	2.6890507568	-1.7162905245	1.0519940880
C3	2.3403415407	-0.5114325234	0.4640971333
C4	0.9971308138	-0.1942081988	0.1867428605
C5	-0.0346403017	-1.1349060082	0.5177187686
C6	0.3567936427	-2.3509779667	1.1149497932

C7	0.5575855834	1.0235537266	-0.4154396581
C8	-0.7834501811	1.3127362226	-0.6797285416
C9	-1.8773065221	0.3973067224	-0.3669639701
C10	-1.4703417139	-0.8963042822	0.2672223333
C11	-0.8268344025	2.6105309807	-1.2795939129
C12	0.4628643239	3.0702855609	-1.3640944399
N13	1.3068861853	2.1063835228	-0.8389014284
O14	-2.3232655445	-1.7601781779	0.5804172906
O15	-3.0627721173	0.6840859617	-0.6153193257
H16	1.9477986961	-3.5917503618	1.8411454079
H17	3.7313731360	-1.9407957291	1.2573481219
H18	3.1236990529	0.2013923106	0.2135025576
H19	-0.4405254848	-3.0451806092	1.3557840288
H20	-1.7207221343	3.1211516920	-1.6016651350
H21	0.8592627675	3.9970853756	-1.7505227748
H22	2.3066391739	2.1825052692	-0.7760113329

#####mol\_double\_reduced#####

22

structure

C1	1.6657537151	-2.6599896652	1.3851145246
C2	2.7056265196	-1.7276695693	1.0590426097
C3	2.3632884457	-0.5242041688	0.4725154008
C4	1.0227501082	-0.1716911837	0.1789309589
C5	-0.0599915450	-1.1235158383	0.5098662892
C6	0.3515804429	-2.3439469892	1.1108069054
C7	0.5952274657	1.0209258635	-0.4105908994
C8	-0.7754715299	1.2882945354	-0.6676868954
C9	-1.8704989516	0.3898682601	-0.3626679573
C10	-1.4784432513	-0.9040221875	0.2699437626
C11	-0.8324826602	2.5936501838	-1.2724826560
C12	0.4444252733	3.0838114617	-1.3723637965
N13	1.3248187436	2.1386784541	-0.8521842777
O14	-2.3567606125	-1.7772111957	0.5849154537
O15	-3.0713491363	0.7059656362	-0.6256143821
H16	1.9184674216	-3.6148046085	1.8484091185
H17	3.7490485948	-1.9625802024	1.2694505644
H18	3.1590111251	0.1851853310	0.2249453727
H19	-0.4602801362	-3.0289038347	1.3456411886
H20	-1.7433885802	3.0840616411	-1.5869101083
H21	0.8146888590	4.0223157153	-1.7668364008
H22	2.3222003395	2.2356123321	-0.7993324837

#####mol92#####

#####mol#####

21

structure

C1	2.2534579518	0.8735634517	2.3946567227
C2	2.7818779991	1.1804374158	1.1407474351
N3	2.1423477659	0.9590942000	-0.0111957280
C4	0.9224416060	0.4093292142	0.0619232050



C5	0.2950727642	0.0608326431	1.2755402899
C6	0.9864528793	0.3035198295	2.4589567225
C7	0.1979571167	0.1536334852	-1.1625898770
C8	-1.0718509102	-0.4089327710	-1.2598826343
C9	-1.8119269192	-0.8063944945	-0.0712383565
C10	-1.0725466744	-0.5516068920	1.2955187112
C11	-1.3972130162	-0.4774899347	-2.6450021211
C12	-0.3248626529	0.0403412819	-3.3325447659
N13	0.6364889286	0.4195564901	-2.4190662633
O14	-1.6176697282	-0.8526931025	2.3306690740
O15	-2.9167592792	-1.3017044613	-0.0600548846
H16	2.8248900203	1.0787774430	3.2911359932
H17	3.7685401039	1.6265052933	1.0562037414
H18	0.5188782621	0.0417307235	3.4008792740
H19	-2.3100114159	-0.8621986523	-3.0694858639
H20	-0.1656243344	0.1703444065	-4.3903653094
H21	1.5366435007	0.8327858064	-2.6123126581

#####mol\_reduced#####

21

structure

C1	2.2224282962	0.8593828962	2.4024006642
C2	2.7870126837	1.1818257187	1.1552039015
N3	2.1704440801	0.9710849638	-0.0040043002
C4	0.9388607041	0.4181100693	0.0359038144
C5	0.2610321390	0.0474872016	1.2433947081
C6	0.9598451711	0.2930204882	2.4371164969
C7	0.2310710387	0.1690552485	-1.1731207910
C8	-1.0434315628	-0.3982899299	-1.2232017258
C9	-1.7857922154	-0.7970833193	-0.0271200963
C10	-1.0834991706	-0.5555561050	1.2762339968
C11	-1.3998307663	-0.4808710160	-2.6056614344
C12	-0.3504764610	0.0290417989	-3.3348191551
N13	0.6415807502	0.4241799300	-2.4594427411
O14	-1.6163180104	-0.8548693787	2.3711023923
O15	-2.9203087725	-1.3008993439	-0.0959981354
H16	2.7771901336	1.0563341167	3.3145483940
H17	3.7786412464	1.6283810385	1.0997359948
H18	0.4678376742	0.0211431633	3.3646583150
H19	-2.3264929455	-0.8738611393	-2.9936784117
H20	-0.2257521196	0.1440526049	-4.4008976293
H21	1.5333120533	0.8350999418	-2.6786100047

#####mol\_double\_reduced#####

21

structure

C1	2.2089946921	0.8519451819	2.4255230413
C2	2.8026250038	1.1881376947	1.1697906914
N3	2.2065127904	0.9868610591	0.0053758374
C4	0.9610614518	0.4297622065	0.0046864403
C5	0.2368870209	0.0371271270	1.2340202208

C6	0.9467927553	0.2873672677	2.4285054000
C7	0.2684838295	0.1860346381	-1.1792130645
C8	-1.0272955355	-0.3926677169	-1.1952557831
C9	-1.7769012486	-0.7933434928	-0.0201399405
C10	-1.0896658765	-0.5587493364	1.2850052784
C11	-1.4035283001	-0.4839112998	-2.5831244170
C12	-0.3769773299	0.0176557420	-3.3461967195
N13	0.6459648981	0.4283733156	-2.5015454676
O14	-1.6414001098	-0.8673165872	2.3951627410
O15	-2.9334873586	-1.3050454602	-0.1206013286
H16	2.7517473252	1.0426030141	3.3517426053
H17	3.8012814332	1.6366246675	1.1381054474
H18	0.4344753315	0.0066678658	3.3466190054
H19	-2.3423650853	-0.8841594110	-2.9401191418
H20	-0.2815478776	0.1199632061	-4.4204122187
H21	1.5284594422	0.8368174041	-2.7506812461

#####mol93#####

#####mol#####

21

structure

C1	2.2293334013	0.8543991176	2.4319325460
C2	2.7819449390	1.1694328480	1.1882732810
N3	2.1671625619	0.9613811635	0.0244448987
C4	0.9414027111	0.4154083297	0.0539172934
C5	0.2927356542	0.0602663977	1.2577406903
C6	0.9629906768	0.2905713805	2.4607405906
C7	0.2502111337	0.1782138053	-1.2031493594
C8	-1.0588022345	-0.4003134606	-1.2592730097
C9	-1.8089019693	-0.7991968088	-0.0757706479
C10	-1.0735654893	-0.5475629623	1.2825697061
C11	-1.4168732244	-0.4858251153	-2.5921086574
N12	-0.3793895287	0.0154929411	-3.3217132901
C13	0.6455602189	0.4253696349	-2.4968863309
O14	-1.6229040675	-0.8484678287	2.3179714203
O15	-2.9165097997	-1.2914183969	-0.0789284728
H16	2.7823022285	1.0490556697	3.3425687417
H17	3.7722981461	1.6127684711	1.1265777036
H18	0.4728624713	0.0211654888	3.3889156402
H19	-2.3170917331	-0.8606244534	-3.0499230399
H20	-0.3630943728	0.0780999148	-4.3271524837
H21	1.5561364779	0.8511455607	-2.8820862758

#####mol\_reduced#####

21

structure

C1	2.2046866217	0.8435162467	2.4325205879
C2	2.7888447046	1.1717188291	1.2012166737
N3	2.1872468183	0.9699806645	0.0286975370
C4	0.9576143442	0.4235880732	0.0350201775
C5	0.2638979162	0.0492373368	1.2270303108

C6	0.9401355321	0.2817886443	2.4389132470
C7	0.2752314568	0.1899127003	-1.2159170875
C8	-1.0367729492	-0.3922712932	-1.2305982397
C9	-1.7837974516	-0.7906750405	-0.0293922992
C10	-1.0879641786	-0.5527118956	1.2599559451
C11	-1.4220380906	-0.4901375593	-2.5557482050
N12	-0.3933816186	0.0095701874	-3.3246503707
C13	0.6462001716	0.4273617651	-2.5270548113
O14	-1.6149386611	-0.8474417390	2.3618708211
O15	-2.9213790516	-1.2914401497	-0.1162627762
H16	2.7432733870	1.0310798982	3.3569677432
H17	3.7826576204	1.6152632023	1.1618051323
H18	0.4269579716	0.0030684009	3.3523751876
H19	-2.3323144943	-0.8707746910	-2.9876486962
H20	-0.3997443938	0.0621481977	-4.3286158765
H21	1.5487713078	0.8509713507	-2.9350990134

#####mol\_double\_reduced#####

21

structure

C1	2.1900713711	0.8362056191	2.4448085250
C2	2.8060037012	1.1789397288	1.2117905134
N3	2.2046937717	0.9777865341	0.0312482387
C4	0.9765765659	0.4331217221	0.0150790638
C5	0.2352016529	0.0372915522	1.2118200649
C6	0.9319164779	0.2780056363	2.4368880463
C7	0.3029488311	0.2028425510	-1.2281577769
C8	-1.0201571307	-0.3861834146	-1.2069938087
C9	-1.7696205577	-0.7850331782	-0.0154026285
C10	-1.0924844786	-0.5550757256	1.2679716968
C11	-1.4280816091	-0.4938450217	-2.5377583992
N12	-0.4089114927	0.0030862980	-3.3348226910
C13	0.6469056220	0.4291611552	-2.5569620426
O14	-1.6287658742	-0.8555014335	2.3969925055
O15	-2.9290273749	-1.2927258950	-0.1507792194
H16	2.7203649703	1.0191686355	3.3821148373
H17	3.8039863663	1.6237167336	1.1865380149
H18	0.4010616089	-0.0083146843	3.3405770393
H19	-2.3469489277	-0.8794436641	-2.9489298461
H20	-0.4316836902	0.0482355001	-4.3384558466
H21	1.5412056559	0.8504248577	-2.9907464024

#####mol94#####

#####mol#####

16

structure

C1	-1.3248398240	2.0425385402	0.0998306220
C2	-0.1302708671	1.2106418777	0.0879844850
C3	-0.1162955636	-0.1778321022	0.0915475541
C4	-1.3789917326	-0.9258390091	0.1084295767
C5	-2.6186917161	-0.0787403124	0.1207869157

C6	-2.5967662537	1.2624024760	0.1169376055
C7	1.2395300291	-0.5903052216	0.0766827828
C8	2.0030949889	0.5613389512	0.0645929413
N9	1.1618027239	1.6441605803	0.0715991865
O10	-1.4568485990	-2.1416947447	0.1125818363
O11	-1.2989148025	3.2648059661	0.0962183419
H12	-3.5490185859	-0.6362219458	0.1332457349
H13	-3.5049001393	1.8551604674	0.1260577390
H14	1.6060815467	-1.6039112546	0.0750809602
H15	3.0733866688	0.6888689157	0.0516414994
H16	1.4258520210	2.6180908165	0.0658738649

#####mol\_reduced#####

16

structure

C1	-1.3369736417	2.0573483257	0.0999450683
C2	-0.1628812874	1.2109690847	0.0883714428
C3	-0.1491961281	-0.1857436048	0.0919532190
C4	-1.3979142209	-0.9422164576	0.1087013259
C5	-2.5792883242	-0.0995380509	0.1203460251
C6	-2.5538399921	1.2855802032	0.1163418104
C7	1.2232569746	-0.5864716475	0.0768517863
C8	1.9864012059	0.5604425935	0.0647626066
N9	1.1374990507	1.6486847923	0.0718582834
O10	-1.4425960991	-2.1986219770	0.1126065989
O11	-1.2538323835	3.3195235421	0.0955902889
H12	-3.5286472052	-0.6296346599	0.1329281516
H13	-3.4810888448	1.8538882196	0.1257299167
H14	1.5882992573	-1.6023968102	0.0752804780
H15	3.0583133895	0.6904889215	0.0517616694
H16	1.3725760368	2.6275089448	0.0664494368

#####mol\_double\_reduced#####

16

structure

C1	-1.3382547232	2.0865305725	0.0998733781
C2	-0.1965539943	1.2170992669	0.0887574341
C3	-0.1824340984	-0.1972974563	0.0923823130
C4	-1.4156924505	-0.9779676565	0.1090138773
C5	-2.5551883332	-0.1254161048	0.1201385639
C6	-2.5204663588	1.3098751573	0.1158700233
C7	1.2011496883	-0.5819774576	0.0770833404
C8	1.9718273534	0.5653192435	0.0649290841
N9	1.1163397265	1.6553879523	0.0721028441
O10	-1.4232427904	-2.2708996437	0.1125802168
O11	-1.2006161805	3.3873263273	0.0947655039
H12	-3.5274042503	-0.6278923930	0.1329373294
H13	-3.4672743000	1.8606261674	0.1255279524
H14	1.5632756176	-1.6030658177	0.0755318339
H15	3.0480779293	0.6943125491	0.0518894315
H16	1.3110992441	2.6438244733	0.0671491595

#####mol95#####

#####mol#####

16

structure

C1	-1.3524422754	2.0693061792	0.1002975064
C2	-0.1149434255	1.2849681575	0.0876258036
C3	-0.1194119629	-0.1453448594	0.0913743842
C4	-1.3618062436	-0.9218390341	0.1081375508
C5	-2.6060999036	-0.0938849866	0.1207388600
C6	-2.6018971319	1.2492514169	0.1172163081
C7	1.1929560167	-0.5632457570	0.0768667927
N8	1.9749786486	0.5632282476	0.0646623902
C9	1.2000007688	1.6946025637	0.0709410182
O10	-1.4128534121	-2.1411613785	0.1119218944
O11	-1.3958402582	3.2889287078	0.0976845726
H12	-3.5319339790	-0.6596088450	0.1331606039
H13	-3.5241650303	1.8208277306	0.1266553312
H14	1.6144136577	-1.5546365088	0.0744213965
H15	2.9826021664	0.5600349916	0.0526878560
H16	1.6276401572	2.6833152485	0.0632940436

#####mol\_reduced#####

16

structure

C1	-1.3756039600	2.0831314666	0.1005251263
C2	-0.1405302888	1.2890600560	0.0879162803
C3	-0.1450197907	-0.1492615692	0.0916854761
C4	-1.3850399471	-0.9355047564	0.1084484764
C5	-2.5687126688	-0.1189861838	0.1203746887
C6	-2.5643591932	1.2741099539	0.1167148523
C7	1.1732660283	-0.5660633129	0.0771057297
N8	1.9618035195	0.5632548464	0.0648332607
C9	1.1803323975	1.6975299401	0.0711821410
O10	-1.3833256843	-2.1943833421	0.1117004913
O11	-1.3660146046	3.3419747106	0.0971687112
H12	-3.5126801464	-0.6595588519	0.1329659231
H13	-3.5049233155	1.8206431194	0.1264476528
H14	1.5926688377	-1.5589134722	0.0746841156
H15	2.9671513010	0.5600609058	0.0528977968
H16	1.6059193151	2.6877198112	0.0635662726

#####mol\_double\_reduced#####

16

structure

C1	-1.3904905774	2.1151457633	0.1006201093
C2	-0.1704380129	1.2984179236	0.0882482836
C3	-0.1749970126	-0.1584493525	0.0920681988
C4	-1.4001535979	-0.9674322049	0.1087061036
C5	-2.5429980700	-0.1473853476	0.1201436774
C6	-2.5384533106	1.3023438976	0.1163367391
C7	1.1525882354	-0.5692901869	0.0773657078

N8	1.9501333304	0.5633123903	0.0649779114
C9	1.1596765249	1.7009066306	0.0714187254
O10	-1.3470642974	-2.2644492030	0.1114374387
O11	-1.3292742414	3.4117968937	0.0965507682
H12	-3.5076877480	-0.6663401809	0.1329339486
H13	-3.4998627681	1.8274080709	0.1263789269
H14	1.5691409636	-1.5661438603	0.0749877334
H15	2.9555022577	0.5600744965	0.0530445900
H16	1.5823667233	2.6951449519	0.0638204406

#####mol96#####

#####mol#####

16

structure

C1	-1.9271520471	1.6367811065	0.1010685151
C2	-0.7455670817	0.9149211282	0.0905155609
C3	-0.7435302070	-0.4788615312	0.0918750611
C4	-1.9229683779	-1.2041892945	0.1038039845
C5	-3.1212083530	-0.4845907069	0.1145055410
C6	-3.1232625415	0.9136533989	0.1131664955
C7	0.6749147661	-0.9528856861	0.0788940103
N8	1.4402920247	0.2211751293	0.0704314344
C9	0.6715225860	1.3930337367	0.0765550725
O10	1.0968961455	2.5209355507	0.0713817785
O11	1.1035141519	-2.0795746865	0.0759761749
H12	-1.9166853132	2.7200046992	0.0999152965
H13	-1.9092714960	-2.2873773547	0.1047335376
H14	-4.0654552907	-1.0165403813	0.1240151775
H15	-4.0690809739	1.4428236666	0.1216662265
H16	2.4495408155	0.2226097077	0.0608373418

#####mol\_reduced#####

16

structure

C1	-1.9375783974	1.6367257271	0.1011547456
C2	-0.7231121351	0.9375790988	0.0902886885
C3	-0.7210107166	-0.5014186412	0.0916937060
C4	-1.9333721623	-1.2041275547	0.1039177065
C5	-3.1253327678	-0.4991084870	0.1145644746
C6	-3.1274369831	0.9281957209	0.1131782415
C7	0.6483005406	-0.9693316711	0.0791441460
N8	1.4077817568	0.2211104618	0.0707379971
C9	0.6448285550	1.4093802270	0.0768122120
O10	1.1276240782	2.5526612005	0.0710939056
O11	1.1342281020	-2.1112782446	0.0756737433
H12	-1.9319488873	2.7230852611	0.1000290907
H13	-1.9245146795	-2.2904650827	0.1049025104
H14	-4.0716239066	-1.0328347546	0.1241027279
H15	-4.0753082857	1.4591296623	0.1216853951
H16	2.4150885507	0.2227689403	0.0611552136

#####mol\_double\_reduced#####

16

structure

C1	-1.9530870313	1.6393372045	0.1013064740
C2	-0.7109301599	0.9689533955	0.0901305635
C3	-0.7088898687	-0.5321820756	0.0915979801
C4	-1.9486063800	-1.2064770893	0.1040384324
C5	-3.1457649852	-0.5157718020	0.1147655350
C6	-3.1478459146	0.9448244748	0.1133680530
C7	0.6281479881	-0.9911897906	0.0793768637
N8	1.3782396224	0.2208412542	0.0710177642
C9	0.6247003707	1.4311561864	0.0769592351
O10	1.1778499912	2.5828617006	0.0705551352
O11	1.1831835288	-2.1418785336	0.0753036053
H12	-1.9558643327	2.7324512271	0.1002679793
H13	-1.9476468921	-2.2995869033	0.1050903038
H14	-4.0943412006	-1.0561195137	0.1243269135
H15	-4.0980679078	1.4823553983	0.1219106426
H16	2.3865867599	0.2236666618	0.0614198917

#####mol97#####

#####mol#####

16

structure

C1	-0.8850681534	2.5015007934	0.0952558181
C2	0.2330157880	1.7385775667	0.0875964552
C3	0.2356997210	0.2526644786	0.0940451109
C4	-0.9206081321	-0.4539879959	0.1084817672
C5	-2.2030598316	0.2543620086	0.1180142420
C6	-2.1826536502	1.8325677574	0.1109258545
C7	1.6281327115	-0.1449327010	0.0821106652
C8	2.3715180406	0.9870233026	0.0698755480
N9	1.5600195564	2.1172660710	0.0729098506
O10	-3.2729889149	-0.3180185851	0.1310503174
O11	-3.2388869292	2.4312201797	0.1187069999
H12	-0.8710721626	3.5849978588	0.0903903188
H13	-0.9451941829	-1.5373503807	0.1134375929
H14	2.0032751273	-1.1549769480	0.0828359361
H15	3.4454726368	1.0982965727	0.0588481535
H16	1.8883435395	3.0675977566	0.0655330523

#####mol\_reduced#####

16

structure

C1	-0.9019913273	2.4626580577	0.0955904514
C2	0.2521100378	1.7081316691	0.0875480442
C3	0.2587550320	0.2668671013	0.0937671092
C4	-0.9491007340	-0.4196267999	0.1086324312
C5	-2.2098331851	0.2707453210	0.1180125849
C6	-2.1894967754	1.8141426624	0.1110717089
C7	1.6440709352	-0.1355939339	0.0819036878
C8	2.4136952421	0.9960542286	0.0694195512

N9	1.5828044333	2.1125995105	0.0727149134
O10	-3.3040033870	-0.3316418615	0.1314023641
O11	-3.2587142981	2.4513259197	0.1187989209
H12	-0.8883101780	3.5497371414	0.0907075664
H13	-0.9855083652	-1.5060401153	0.1137201511
H14	2.0168322981	-1.1497179356	0.0826535711
H15	3.4874729910	1.1106009646	0.0583738578
H16	1.8897029920	3.0682954108	0.0655375196

#####mol\_double\_reduced#####

16

structure

C1	-0.9120308455	2.4408831672	0.0957956212
C2	0.2777602107	1.6890050161	0.0873867564
C3	0.2832064990	0.2710394878	0.0935182670
C4	-0.9758199773	-0.4079030897	0.1088469253
C5	-2.2270009397	0.2618411132	0.1182161312
C6	-2.1958899067	1.8106588049	0.1111538611
C7	1.6591324690	-0.1273698724	0.0817379330
C8	2.4676983449	1.0073296691	0.0688328459
N9	1.6061499744	2.1101146646	0.0724931996
O10	-3.3512409562	-0.3357001424	0.1318562284
O11	-3.2779923360	2.4700723028	0.1189050018
H12	-0.8976937594	3.5353254021	0.0908842095
H13	-1.0125319040	-1.5012447047	0.1139606572
H14	2.0281225023	-1.1492125617	0.0825650825
H15	3.5423470292	1.1292748450	0.0577277095
H16	1.8905489681	3.0732078751	0.0654929722

#####mol98#####

#####mol#####

16

structure

C1	-0.6905309229	1.9649574117	0.0936540837
C2	0.4746170954	1.1092249611	0.0857328648
C3	0.4397523435	-0.2834621121	0.0944054464
C4	-0.8329180526	-0.9824789446	0.1127710718
C5	-1.9976676294	-0.3026652499	0.1218064931
C6	-2.0480532604	1.1757192592	0.1136674439
C7	1.7824627557	-0.7335862560	0.0820918862
C8	2.5874806282	0.3956489797	0.0663915890
N9	1.7867471542	1.4993788421	0.0687619778
O10	-0.6624363416	3.1801760706	0.0860109347
O11	-3.0889373867	1.7953816372	0.1218034786
H12	-0.8307372032	-2.0677132260	0.1191457210
H13	-2.9575750582	-0.8048486865	0.1355186714
H14	2.1308135028	-1.7545377847	0.0842744219
H15	3.6618193477	0.4845296400	0.0538729499
H16	2.0844776847	2.4632889809	0.0597035813

#####mol\_reduced#####

16



structure

C1	-0.7168187592	1.9385789969	0.0941659630
C2	0.4329723940	1.0712702644	0.0864487810
C3	0.4352527882	-0.3323668667	0.0947671344
C4	-0.8239296110	-1.0042172559	0.1128429807
C5	-1.9746596162	-0.2534099297	0.1212605634
C6	-2.0250128998	1.2067177141	0.1131732634
C7	1.8102071864	-0.7389148199	0.0817988495
C8	2.5815064034	0.4054324861	0.0663660804
N9	1.7422431492	1.4960791321	0.0692706623
O10	-0.5912360545	3.1885512448	0.0853269159
O11	-3.1194125760	1.8213129745	0.1217974191
H12	-0.8678397349	-2.0906753397	0.1197778883
H13	-2.9492902051	-0.7352586970	0.1350154913
H14	2.1908812323	-1.7510877233	0.0835500336
H15	3.6546848540	0.5235999595	0.0536603396
H16	1.9802879857	2.4740448491	0.0607911555

#####mol\_double\_reduced#####

16

structure

C1	-0.7169941921	1.9281231168	0.0942436508
C2	0.3953368949	1.0472116915	0.0870261103
C3	0.4304109209	-0.3829188631	0.0951271011
C4	-0.8129004127	-1.0367723860	0.1129254699
C5	-1.9657601648	-0.2230364455	0.1209849224
C6	-2.0276913356	1.2256484077	0.1130743842
C7	1.8288287318	-0.7466742595	0.0816279538
C8	2.5805715477	0.4153034579	0.0663123837
N9	1.7201845593	1.4945361641	0.0695441970
O10	-0.5333893966	3.2085627212	0.0845903036
O11	-3.1488236383	1.8500699491	0.1218961236
H12	-0.8925373880	-2.1268692164	0.1202977560
H13	-2.9530391681	-0.6963341149	0.1348351423
H14	2.2428291766	-1.7517956724	0.0829533818
H15	3.6568392594	0.5467373374	0.0534746964
H16	1.9017003363	2.4846344924	0.0616235141

#####mol99#####

#####mol#####

16

structure

C1	-0.7361019630	1.9849231177	0.0955490351
C2	0.4902044067	1.1932358875	0.0857245213
C3	0.4251660933	-0.1986665774	0.0935139219
C4	-0.7927349510	-0.9654369392	0.1111501689
C5	-1.9828560873	-0.3287641214	0.1214256135
C6	-2.0731905646	1.1472261239	0.1150512073
N7	1.7094334441	-0.6661133382	0.0813923065
C8	2.5898211605	0.3950949350	0.0660911511
C9	1.8614462358	1.5626137443	0.0683859678

O10	-0.7876957707	3.1947255225	0.0898919193
O11	-3.1355593296	1.7293178902	0.1242828141
H12	-0.7416531546	-2.0502078634	0.1160277260
H13	-2.9233735522	-0.8658020407	0.1347692687
H14	1.9764135057	-1.6378511869	0.0833006406
H15	3.6548345897	0.2309588752	0.0549228636
H16	2.2553163645	2.5658297203	0.0588640219

#####mol\_reduced#####

16

structure

C1	-0.7626393524	1.9621833781	0.0959927132
C2	0.4510239051	1.1602860754	0.0863515293
C3	0.4229607539	-0.2447182355	0.0937829986
C4	-0.7786334838	-0.9894482565	0.1111378948
C5	-1.9622909581	-0.2758528115	0.1209447634
C6	-2.0542592443	1.1714160420	0.1146836001
N7	1.7369004234	-0.6827638707	0.0811511822
C8	2.5902826656	0.4141125527	0.0659794976
C9	1.8275673083	1.5540144998	0.0688245128
O10	-0.7421856669	3.2068948118	0.0893957826
O11	-3.1672353009	1.7546926644	0.1243888482
H12	-0.7687052164	-2.0767537339	0.1165098538
H13	-2.9173706576	-0.7949382466	0.1343813871
H14	2.0255516108	-1.6452071453	0.0827508398
H15	3.6615011324	0.2792276740	0.0545757077
H16	2.1878319088	2.5713286529	0.0596122211

#####mol\_double\_reduced#####

16

structure

C1	-0.7676441736	1.9511130500	0.0961498235
C2	0.4250191972	1.1370148574	0.0867832706
C3	0.4210431274	-0.2981977765	0.0940927332
C4	-0.7606206212	-1.0141996261	0.1110847471
C5	-1.9659209819	-0.2386771836	0.1207826676
C6	-2.0709923443	1.1869135361	0.1147580647
N7	1.7734234257	-0.7060185453	0.0808607750
C8	2.6035753741	0.4260737188	0.0657370800
C9	1.8049894080	1.5423048789	0.0691212230
O10	-0.7094950244	3.2225374865	0.0890513700
O11	-3.1988644423	1.8020148287	0.1243986262
H12	-0.7847815998	-2.1071253561	0.1168972366
H13	-2.9284776109	-0.7599341823	0.1342881814
H14	2.0881934264	-1.6593595449	0.0821160688
H15	3.6826003376	0.3212172068	0.0540611720
H16	2.1375633916	2.5728859957	0.0601437309

#####mol100#####

#####mol#####

9

structure

C1	-0.3699542018	1.3455014927	0.0862653798
C2	0.0935042242	0.0620225826	0.0718516443
S3	1.8258603759	0.0113265520	0.0667279635
C4	1.9209279232	1.7417446276	0.0842310956
C5	0.6808651295	2.3113911312	0.0933838655
H6	-1.4221603029	1.5972909276	0.0916553654
H7	-0.4705779796	-0.8575452625	0.0639070261
H8	2.8846888866	2.2265347494	0.0866372354
H9	0.5183525539	3.3809847203	0.1048031408

#####mol\_reduced#####

9

structure

C1	-0.3836615689	1.3843620297	0.0866841773
C2	0.0548707028	0.0451187289	0.0717534233
S3	1.8550925692	-0.0204656476	0.0663618270
C4	1.9410193734	1.7788436250	0.0845315264
C5	0.6432806720	2.3282760403	0.0936400474
H6	-1.4380561332	1.6492711232	0.0922184152
H7	-0.5161861197	-0.8697940638	0.0638384651
H8	2.9007275519	2.2709795164	0.0869879636
H9	0.4679609405	3.4011673244	0.1051286329

#####mol101#####

#####mol#####

9

structure

C1	-0.4029917771	1.3734321842	0.0874350575
C2	0.2055918111	0.1598358614	0.0725871410
O3	1.5600787996	0.3056501631	0.0694875263
C4	1.8123922268	1.6443340801	0.0827070962
C5	0.6505823214	2.3468069966	0.0940696411
H6	-1.4654344219	1.5573496281	0.0930021305
H7	-0.1568350102	-0.8538816576	0.0631623984
H8	2.8516072596	1.9255731434	0.0821123059
H9	0.5511107452	3.4204006036	0.1057039788

#####mol\_reduced#####

9

structure

C1	-0.3998637054	1.3765128729	0.0888520854
C2	0.2022898786	0.1643443587	0.0724578606
O3	1.5671958964	0.2979545290	0.0675577516
C4	1.8081671857	1.6479934192	0.0821402797
C5	0.6472485283	2.3439458640	0.0954135150
H6	-1.4951113542	1.5500873839	0.0934859495
H7	-0.1821287904	-0.8696950558	0.0664102217
H8	2.8694160281	1.9494997572	0.0856255669
H9	0.5606665487	3.4494276865	0.1067967930

#####mol102#####

#####mol#####

15

structure

S1	0.3107998286	-1.6487680493	-2.0850724991
C2	0.5247363402	0.0585410195	-1.8574149904
C3	0.2287478705	0.4203835791	-0.5775546468
C4	-0.1783140361	-0.6884211956	0.2385218898
C5	-0.1830863260	-1.8721554194	-0.4362512675
O6	0.2897844193	1.6990832448	-0.0960080600
C7	0.2905383459	1.7435719476	1.3368581833
C8	-0.7739976152	0.8216076077	1.9072029983
O9	-0.5077634699	-0.5430218076	1.5579960124
H10	0.8535348149	0.6931218846	-2.6636367738
H11	-0.4480501879	-2.8459943566	-0.0591247852
H12	0.0924825600	2.7809389874	1.6087035994
H13	1.2794427088	1.4545572131	1.7131487226
H14	-1.7629413366	1.1110160520	1.5312790568
H15	-0.7789617302	0.8610189167	2.9970180970

#####mol\_reduced#####

15

structure

S1	0.3119320530	-1.6680950547	-2.1111854780
C2	0.7492139325	0.0685983834	-1.8433236663
C3	0.2910809270	0.3866224274	-0.5387564390
C4	-0.2377781065	-0.6529747257	0.2047339963
C5	-0.4072956185	-1.8934286245	-0.4635871272
O6	0.3616790604	1.7058063548	-0.0527471773
C7	0.3213040494	1.7279458637	1.3586798988
C8	-0.8052359212	0.8420302014	1.8903830869
O9	-0.5829104540	-0.5132898356	1.5624776884
H10	0.5373690619	0.7329098261	-2.6796150654
H11	-0.1408077840	-2.8267264895	0.0303090485
H12	0.1650239674	2.7701164390	1.6610744691
H13	1.2768355835	1.3727783949	1.7776547382
H14	-1.7596203815	1.1909208460	1.4635603894
H15	-0.8593229955	0.9055848065	2.9835868447

#####mol103#####

#####mol#####

21

structure

C1	-3.3017477918	0.5092477889	-0.7463993768
C2	-2.8442465863	-0.4284079002	-1.6720046037
C3	-1.5212218603	-0.8615748102	-1.6446904935
C4	-0.6444991324	-0.3537968963	-0.6831799289
C5	-1.1032204661	0.5966995344	0.2574878974
C6	-2.4314268998	1.0177007735	0.2135515103
C7	0.7427368367	-0.7462805304	-0.5819328570
C8	1.6672642153	-0.2971238727	0.3288761401
C9	1.3065540513	0.6835814398	1.3456339579
C10	-0.1899360994	1.1622304215	1.3026700904
C11	2.8952786353	-0.9736892514	0.0275020970

C12	2.6232106813	-1.7725268736	-1.0318119918
O13	1.3076061346	-1.6447823153	-1.4176412615
O14	-0.5652343390	1.9748248894	2.1146496137
O15	2.0580897479	1.1298187951	2.1821575553
H16	-4.3325632692	0.8417006907	-0.7738028402
H17	-3.5210254332	-0.8251555292	-2.4199904888
H18	-1.1632285935	-1.5894126085	-2.3621804342
H19	-2.7609170615	1.7465335623	0.9440291057
H20	3.8378608031	-0.8674537998	0.5386654129
H21	3.2084451765	-2.4637527423	-1.6132386803

#####mol\_reduced#####

21

structure

C1	-3.2879135159	0.5256555476	-0.7208692929
C2	-2.8595643252	-0.4232684337	-1.6719140926
C3	-1.5488312746	-0.8645538463	-1.6596744391
C4	-0.6356603000	-0.3752780310	-0.7053562195
C5	-1.0582405084	0.5899344183	0.2676710874
C6	-2.4013826145	1.0137496143	0.2212456495
C7	0.7245295501	-0.7650525041	-0.6118494046
C8	1.6185303718	-0.2837387863	0.3250663867
C9	1.2628776752	0.6962241373	1.3430814705
C10	-0.1649551787	1.1548824592	1.3038811004
C11	2.8650415784	-0.9451846305	0.0493165744
C12	2.6413743914	-1.7603284160	-1.0098866006
O13	1.3379541129	-1.6761406085	-1.4427568328
O14	-0.5940716765	1.9944285951	2.1253412175
O15	2.0883870613	1.1137841985	2.1761083790
H16	-4.3171757801	0.8725854421	-0.7301643331
H17	-3.5553787741	-0.8069337629	-2.4120018206
H18	-1.2043837313	-1.5944962938	-2.3853186266
H19	-2.7031207659	1.7435264267	0.9641499654
H20	3.7899324226	-0.8101739660	0.5876508214
H21	3.2651589940	-2.4422803000	-1.5646291433

#####mol\_double\_reduced#####

21

structure

C1	-3.2986781059	0.5442490176	-0.7030856196
C2	-2.8824990513	-0.4207064657	-1.6780116727
C3	-1.5799308245	-0.8685799988	-1.6770208425
C4	-0.6239402098	-0.4020603030	-0.7325885692
C5	-1.0361955673	0.5934794050	0.2808028535
C6	-2.3896234989	1.0122842197	0.2242349148
C7	0.7038788899	-0.7835053333	-0.6426409245
C8	1.5922595872	-0.2732016759	0.3265778042
C9	1.2550186939	0.6963908130	1.3401540225
C10	-0.1687344370	1.1604897126	1.3090069303
C11	2.8486733755	-0.9265749031	0.0647350873
C12	2.6686602242	-1.7556627808	-0.9932807473

O13	1.3714943014	-1.7103222636	-1.4700070228
O14	-0.5957032867	2.0157338136	2.1501152830
O15	2.1086814760	1.1110080202	2.1817021466
H16	-4.3283143725	0.9032550996	-0.6983038481
H17	-3.5912961302	-0.7981111798	-2.4157716305
H18	-1.2544644103	-1.6020717564	-2.4144604045
H19	-2.6707672941	1.7442970340	0.9781561561
H20	3.7602610263	-0.7688178010	0.6249663440
H21	3.3278807229	-2.4293642140	-1.5235333414

#####mol104#####

#####mol#####

21

structure

C1	-3.3780150326	-0.3869214180	-0.7162626585
C2	-2.7573911397	-1.5626788207	-1.1373809940
C3	-1.3842095865	-1.7277413783	-0.9884939855
C4	-0.6028235510	-0.7184614914	-0.4146676330
C5	-1.2353919172	0.4727203313	0.0107243299
C6	-2.6142756764	0.6237230259	-0.1447878936
C7	0.8397461405	-0.8371763554	-0.2341732804
C8	1.6451559400	0.1379150931	0.3252009690
C9	1.0829266343	1.4087577929	0.7956773839
C10	-0.4578637755	1.5862517618	0.6285658796
C11	3.0235869534	-0.2275669333	0.3850079253
C12	3.2519270448	-1.4667504492	-0.1243065594
S13	1.7882066050	-2.2208032558	-0.6912569359
O14	-0.9747309063	2.6141157946	1.0015832498
O15	1.7411098832	2.2958826866	1.2917006229
H16	-4.4477868015	-0.2615468109	-0.8334558673
H17	-3.3449202558	-2.3563548161	-1.5843484796
H18	-0.9184525212	-2.6482123058	-1.3214583156
H19	-3.0653514027	1.5489989992	0.1925198380
H20	3.7858914124	0.4210296871	0.7928950379
H21	4.1861564210	-1.9999146488	-0.2093916770

#####mol\_reduced#####

21

structure

C1	-3.3694127748	-0.3594386700	-0.7042882902
C2	-2.7717397716	-1.5590196279	-1.1394868942
C3	-1.4088772791	-1.7389163327	-0.9975815806
C4	-0.5934978782	-0.7408661230	-0.4225083344
C5	-1.1966680205	0.4801511253	0.0202560356
C6	-2.5888960960	0.6301112060	-0.1387675846
C7	0.8182083277	-0.8624350762	-0.2477851862
C8	1.5968464950	0.1435527694	0.3195590965
C9	1.0438134077	1.4132341701	0.7908671810
C10	-0.4333918948	1.5865764009	0.6328187218
C11	2.9847087305	-0.2062369862	0.3864929611
C12	3.2588828518	-1.4377951988	-0.1116065965

S13	1.8164916983	-2.2494797681	-0.6963220464
O14	-1.0045501864	2.6315641807	1.0049400656
O15	1.7724151305	2.2899906979	1.2928652376
H16	-4.4401625674	-0.2155902014	-0.8142560494
H17	-3.3780935701	-2.3415409725	-1.5855194931
H18	-0.9503027282	-2.6644449717	-1.3339652873
H19	-3.0145434454	1.5654235330	0.2068703512
H20	3.7202537593	0.4703210363	0.8008760298
H21	4.2114033560	-1.9416411344	-0.1824442054

#####mol\_double\_reduced#####

21

structure

C1	-3.3847335407	-0.3355681662	-0.6967561004
C2	-2.7927215559	-1.5581004321	-1.1435101148
C3	-1.4378086281	-1.7514050789	-1.0085286141
C4	-0.5786571217	-0.7686119241	-0.4324812918
C5	-1.1810408767	0.4945216107	0.0287612894
C6	-2.5801221123	0.6349658442	-0.1355516163
C7	0.7928932062	-0.8887130412	-0.2629422074
C8	1.5737699182	0.1535217576	0.3202617595
C9	1.0397114358	1.4153191343	0.7908430002
C10	-0.4390722166	1.5939358053	0.6349393976
C11	2.9597581910	-0.1919814842	0.3876107799
C12	3.2819359570	-1.4183050403	-0.0995111833
S13	1.8488288207	-2.2869560200	-0.7051180409
O14	-1.0087379492	2.6601073764	1.0165765007
O15	1.7811496158	2.3056723809	1.3002631217
H16	-4.4577076446	-0.1766784269	-0.8003408497
H17	-3.4118827099	-2.3362205389	-1.5903898118
H18	-0.9924806605	-2.6853465795	-1.3513759511
H19	-2.9892107438	1.5789977895	0.2168911543
H20	3.6746385531	0.5081202942	0.8073200726
H21	4.2519234789	-1.8944150809	-0.1560263503

#####mol105#####

#####mol#####

20

structure

C1	-2.6787018806	0.1869793303	2.0739905166
C2	-2.5036836556	1.4223114315	1.4496980082
N3	-1.5338623664	1.6838915313	0.5699752532
C4	-0.6878227105	0.6911426229	0.2807861671
C5	-0.7712451208	-0.5979381299	0.8528067477
C6	-1.7936537237	-0.8393004772	1.7669300866
C7	0.3888567608	0.9096370967	-0.6677550288
C8	1.3292133798	-0.0139234682	-1.0605151012
C9	1.3349110659	-1.3745373552	-0.5331676289
C10	0.1967162694	-1.6855793146	0.5031167350
C11	2.1782544631	0.6523225277	-2.0017224047
C12	1.6887234582	1.9132186130	-2.1022231668

O13	0.5946119588	2.0839448285	-1.2918664234
O14	0.1265562294	-2.7873247098	0.9926356934
O15	2.1280686151	-2.2360875647	-0.8337571742
H16	-3.4874322219	0.0412144993	2.7791120111
H17	-3.1772261337	2.2463133336	1.6665579298
H18	-1.8715806156	-1.8228716676	2.2148128675
H19	3.0266882296	0.2358171784	-2.5190088499
H20	1.9773208964	2.7794760214	-2.6721855938

#####mol\_reduced#####

20

structure

C1	-2.6603563658	0.1542452868	2.0722630503
C2	-2.5144382720	1.4135167822	1.4619959614
N3	-1.5634642088	1.7043870880	0.5857981695
C4	-0.6871270570	0.7253230013	0.2668267120
C5	-0.7337348124	-0.5983989078	0.8228001603
C6	-1.7629728444	-0.8452440384	1.7445744130
C7	0.3658606209	0.9436501474	-0.6627463632
C8	1.2896384591	-0.0207994610	-1.0259752808
C9	1.2998191156	-1.3814498921	-0.5017914222
C10	0.2150257940	-1.6805343943	0.4860620018
C11	2.1613066445	0.6158821215	-1.9738154607
C12	1.7105280902	1.8874124208	-2.1098773737
O13	0.6130996826	2.1219867698	-1.3218892775
O14	0.1057651887	-2.8077681655	1.0158854198
O15	2.1491360285	-2.2191134276	-0.8557538692
H16	-3.4631939307	-0.0163723225	2.7825358578
H17	-3.2072856934	2.2194825846	1.7015942538
H18	-1.8127352623	-1.8398548568	2.1740845652
H19	3.0030974092	0.1596614254	-2.4700878674
H20	2.0377979503	2.7275986432	-2.7008355374

#####mol\_double\_reduced#####

20

structure

C1	-2.6626436461	0.1280923605	2.0840376330
C2	-2.5323258116	1.4123984457	1.4768836304
N3	-1.5990079117	1.7301385475	0.6044576077
C4	-0.6869965550	0.7666952276	0.2506662675
C5	-0.7141512219	-0.6080542688	0.8109177007
C6	-1.7478533059	-0.8491292783	1.7336683276
C7	0.3395692131	0.9769494476	-0.6546424441
C8	1.2685698194	-0.0311907930	-1.0050722737
C9	1.2947685466	-1.3802079986	-0.4981895721
C10	0.2155519364	-1.6880805611	0.4887427946
C11	2.1522466467	0.5908755331	-1.9570377320
C12	1.7360297175	1.8701282638	-2.1237553299
O13	0.6312612981	2.1627079172	-1.3524022572
O14	0.1128543710	-2.8381645871	1.0223409782
O15	2.1677031947	-2.2224322981	-0.8692312863



H16	-3.4625758885	-0.0617698025	2.7991705953
H17	-3.2433741708	2.2060863614	1.7360746155
H18	-1.7768622440	-1.8539661003	2.1502785667
H19	2.9891144891	0.1027631417	-2.4371014941
H20	2.0972839815	2.6875932361	-2.7331045229

#####mol106#####

#####mol#####

20

structure

C1	-2.7034089899	0.0933274901	2.1132788550
C2	-2.5632620166	1.3317394483	1.4849152728
N3	-1.6025940102	1.6122379632	0.6031081310
C4	-0.7256047601	0.6443815712	0.3087144176
C5	-0.7781739086	-0.6410939470	0.8869845166
C6	-1.7918768400	-0.9077962426	1.8054345124
C7	0.3287067802	0.9330047244	-0.6509228135
C8	1.2988588392	0.0306678456	-1.0471900004
C9	1.3317225327	-1.3338150560	-0.5048827433
C10	0.2179320162	-1.6930486581	0.5328402008
C11	2.2084990417	0.5775445100	-1.9991067969
C12	1.9119568526	1.8721859206	-2.3025098264
S13	0.5199989493	2.4597406888	-1.4396608785
O14	0.1902815654	-2.7998811476	1.0174311170
O15	2.1531761458	-2.1673761179	-0.8125863041
H16	-3.5056504417	-0.0728608449	2.8212148921
H17	-3.2570753699	2.1390924733	1.7003025847
H18	-1.8425717651	-1.8917207936	2.2564526859
H19	3.0309387853	0.0167581348	-2.4200163971
H20	2.4248771403	2.5320963428	-2.9855127340

#####mol\_reduced#####

20

structure

C1	-2.6869416826	0.0597778829	2.1145587777
C2	-2.5754949696	1.3203098056	1.4997083672
N3	-1.6338400538	1.6290365137	0.6208746711
C4	-0.7290107288	0.6753882133	0.2982758711
C5	-0.7449511192	-0.6414606550	0.8606343706
C6	-1.7636965725	-0.9154137131	1.7863336947
C7	0.3019658800	0.9598897861	-0.6411318778
C8	1.2605621167	0.0201814872	-1.0122838557
C9	1.2996313074	-1.3423751042	-0.4754216946
C10	0.2349267692	-1.6887583076	0.5173253358
C11	2.1872261353	0.5470531576	-1.9691852662
C12	1.9335787592	1.8387382039	-2.3056640468
S13	0.5383289931	2.4911715890	-1.4678276215
O14	0.1707621816	-2.8198192261	1.0406049627
O15	2.1724084872	-2.1548447768	-0.8322102092
H16	-3.4828684701	-0.1296341021	2.8274270337
H17	-3.2872289192	2.1097736359	1.7371170164

H18	-1.7856483626	-1.9098241969	2.2188118650
H19	2.9981298377	-0.0493138842	-2.3656915042
H20	2.4743424353	2.4677298973	-2.9977419750

#####mol\_double\_reduced#####

20

structure

C1	-2.6889256491	0.0307850752	2.1309740639
C2	-2.5921953396	1.3133721866	1.5195674250
N3	-1.6710987325	1.6499886648	0.6434134417
C4	-0.7313663162	0.7120248277	0.2845527462
C5	-0.7291626817	-0.6510559039	0.8520855954
C6	-1.7492025546	-0.9225402757	1.7783785911
C7	0.2700468422	0.9853759707	-0.6280870224
C8	1.2439395503	0.0063997501	-0.9922893591
C9	1.2982742487	-1.3438498511	-0.4718654698
C10	0.2339889587	-1.6960312847	0.5205297733
C11	2.1753537264	0.5266615925	-1.9474954561
C12	1.9630537327	1.8157961275	-2.3193368753
S13	0.5517835943	2.5290839080	-1.5012074888
O14	0.1764960307	-2.8473897247	1.0455581355
O15	2.1878953586	-2.1675730667	-0.8346642904
H16	-3.4806268022	-0.1768960936	2.8490375759
H17	-3.3204140580	2.0903705904	1.7780522964
H18	-1.7507506876	-1.9265910561	2.1974465421
H19	2.9791985368	-0.0989016085	-2.3212560015
H20	2.5290461568	2.4179363580	-3.0185981110

#####mol107#####

#####mol#####

20

structure

C1	-3.4054634304	0.0551086958	-0.0445582049
C2	-2.9403166447	1.3694282301	0.0551485782
N3	-1.6510911924	1.7013305808	0.0969740395
C4	-0.7504174709	0.7092176433	0.0395398590
C5	-1.1123549068	-0.6510946921	-0.0619151245
C6	-2.4731029440	-0.9676431924	-0.1037127733
C7	0.6643491107	1.0480704591	0.0836719631
C8	1.6963778859	0.0462690416	0.0273497629
C9	1.4176435238	-1.3858464167	-0.0781172336
C10	-0.1032802982	-1.7532604977	-0.1255558016
C11	2.8828174016	0.7177917071	0.0917864876
O12	2.6576606749	2.0474942744	0.1828336313
C13	1.3034320649	2.2440052336	0.1775118313
O14	-0.4249017896	-2.9153949242	-0.2122065547
O15	2.2537406186	-2.2576920564	-0.1281460052
H16	-4.4688002080	-0.1474572791	-0.0740151299
H17	-3.6434537073	2.1962036708	0.1037296517
H18	-2.7618596360	-2.0090611209	-0.1815844317
H19	3.9106374652	0.3975402638	0.0837391753

H20 0.9654218352 3.2625305106 0.2449283324  
#####mol\_reduced#####

20

structure

C1	-3.3872811853	0.0394359756	-0.0452419485
C2	-2.9544947923	1.3682574717	0.0548745211
N3	-1.6677094726	1.7162178100	0.0976790048
C4	-0.7502235250	0.7361842456	0.0413307352
C5	-1.0700143841	-0.6488421625	-0.0612235479
C6	-2.4403027780	-0.9675387701	-0.1031369383
C7	0.6563474496	1.0742642727	0.0853548132
C8	1.6595825212	0.0384250527	0.0263216163
C9	1.3651605449	-1.3999419717	-0.0798020925
C10	-0.0743960005	-1.7476731330	-0.1249022946
C11	2.8618011899	0.6840699674	0.0892505834
O12	2.6731908689	2.0400356739	0.1826351038
C13	1.3260350406	2.2590630640	0.1788969045
O14	-0.4679773175	-2.9354868986	-0.2145999199
O15	2.2827766330	-2.2400969782	-0.1262842327
H16	-4.4494770989	-0.1845312017	-0.0760172296
H17	-3.6747777931	2.1828906463	0.1023490823
H18	-2.7024473153	-2.0163881242	-0.1810612110
H19	3.8811436574	0.3414098210	0.0795579914
H20	1.0055562697	3.2839746729	0.2469387607

#####mol\_double\_reduced#####

20

structure

C1	-3.3835688603	0.0243183781	-0.0462681857
C2	-2.9739420515	1.3769610436	0.0551785328
N3	-1.6770086698	1.7284192436	0.0983869898
C4	-0.7511736242	0.7622828814	0.0431642639
C5	-1.0374765942	-0.6593783461	-0.0614526548
C6	-2.4357368816	-0.9716774250	-0.1033161992
C7	0.6480627431	1.0997121142	0.0870242074
C8	1.6322596140	0.0318813690	0.0254006807
C9	1.3433569111	-1.3997435241	-0.0801914991
C10	-0.0780456467	-1.7545239075	-0.1253691585
C11	2.8553204178	0.6647685227	0.0877737115
O12	2.6942418125	2.0396848266	0.1829631863
C13	1.3458475179	2.2734079896	0.1802409861
O14	-0.4888263559	-2.9675624407	-0.2170025793
O15	2.3101755561	-2.2244151485	-0.1249708662
H16	-4.4492243791	-0.2131659673	-0.0780917315
H17	-3.7048540186	2.1864654640	0.1021188522
H18	-2.6795733980	-2.0267322731	-0.1814107968
H19	3.8691832438	0.3052630722	0.0768483099
H20	1.0408092714	3.3052283196	0.2490418080

#####mol108#####

#####mol#####

20

structure

C1	-3.4194226287	0.0427366026	-0.0356347662
C2	-2.9478360408	1.3556425095	0.0514979332
N3	-1.6573263595	1.6810194522	0.0862534086
C4	-0.7571055244	0.6877269071	0.0344766700
C5	-1.1281301066	-0.6696090838	-0.0543032937
C6	-2.4898724977	-0.9824477972	-0.0891137938
C7	0.6623672251	1.0448650757	0.0726943415
C8	1.6906923235	0.0434545285	0.0217882930
C9	1.3909981324	-1.3945492302	-0.0712916960
C10	-0.1231927361	-1.7702470969	-0.1115577590
C11	2.9527280648	0.5774332297	0.0692585982
S12	2.9035855870	2.2935796103	0.1752188432
C13	1.1727524975	2.3104542399	0.1573405895
O14	-0.4418761180	-2.9342912486	-0.1874983627
O15	2.2278449183	-2.2663900482	-0.1164149097
H16	-4.4833780536	-0.1569326644	-0.0600305161
H17	-3.6463101960	2.1867899213	0.0954764354
H18	-2.7819401781	-2.0235521135	-0.1573235363
H19	3.8889298042	0.0415039369	0.0465760144
H20	0.6225656859	3.2361457456	0.2091376782

#####mol\_reduced#####

20

structure

C1	-3.4012743997	0.0295616359	-0.0364217871
C2	-2.9620544573	1.3570169978	0.0513715265
N3	-1.6743083698	1.6986326881	0.0871361523
C4	-0.7583325270	0.7169605082	0.0361934631
C5	-1.0866534916	-0.6634811649	-0.0536109397
C6	-2.4571996828	-0.9800892054	-0.0888131930
C7	0.6526762201	1.0709303391	0.0740971463
C8	1.6541745290	0.0346876233	0.0207663644
C9	1.3422469862	-1.4080781118	-0.0726183870
C10	-0.0933562282	-1.7617618674	-0.1108963446
C11	2.9279440818	0.5470546634	0.0667979544
S12	2.9166895918	2.2781333703	0.1751770060
C13	1.1861055746	2.3306446836	0.1584273322
O14	-0.4845182931	-2.9494842137	-0.1894107420
O15	2.2566166443	-2.2520552039	-0.1148850267
H16	-4.4641062647	-0.1909858642	-0.0621323674
H17	-3.6780147914	2.1755654309	0.0944425985
H18	-2.7217372959	-2.0289245028	-0.1572715208
H19	3.8499273937	-0.0109651688	0.0419831929
H20	0.6506298849	3.2649462735	0.2103033859

#####mol\_double\_reduced#####

20

structure

C1	-3.3976054252	0.0213933496	-0.0369474553
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C2	-2.9824585924	1.3663895459	0.0521056408
N3	-1.6788255711	1.7101390681	0.0883240338
C4	-0.7636925309	0.7384614676	0.0378317937
C5	-1.0578205319	-0.6698024974	-0.0535248992
C6	-2.4552050348	-0.9834431792	-0.0891845345
C7	0.6472862974	1.0862925132	0.0752358158
C8	1.6319394660	0.0231155661	0.0200191108
C9	1.3258876704	-1.4094013993	-0.0724669172
C10	-0.0931283142	-1.7625129058	-0.1107515394
C11	2.9249687762	0.5314122918	0.0657657942
S12	2.9315191082	2.2783199979	0.1741943419
C13	1.1905376636	2.3406089823	0.1590785509
O14	-0.5087443007	-2.9708795195	-0.1910232447
O15	2.2811310496	-2.2457901342	-0.1136193954
H16	-4.4642193417	-0.2106654673	-0.0637040127
H17	-3.7056255554	2.1818028267	0.0950896755
H18	-2.7047118099	-2.0368792440	-0.1581520346
H19	3.8405491509	-0.0361142638	0.0405735931
H20	0.6581223471	3.2778591707	0.2114475617

#####mol109#####

#####mol#####

20

structure

C1	-3.4047990250	0.1109577504	0.1927467551
C2	-2.9066772976	1.4004748337	0.3754670550
N3	-1.6061474068	1.7063173569	0.3580378482
C4	-0.7400747500	0.7086855982	0.1524887391
C5	-1.1383839135	-0.6300569861	-0.0431767040
C6	-2.5001392489	-0.9217604941	-0.0204484547
C7	0.6872086396	1.0166381145	0.1287827368
C8	1.6389780051	0.0448560444	-0.0770487953
C9	1.3879626732	-1.3663132497	-0.2919164124
C10	-0.1410772086	-1.7237745014	-0.2707348653
O11	2.8834919132	0.5930889364	-0.0527104614
C12	2.7125130082	1.9195882257	0.1700986814
C13	1.3925000496	2.2425727477	0.2902421517
O14	-0.4745681321	-2.8720929031	-0.4384513427
O15	2.2178339798	-2.2267291314	-0.4735896824
H16	-4.4718834245	-0.0714381908	0.2180767091
H17	-3.5849894697	2.2317032276	0.5445712176
H18	-2.8182719022	-1.9467900969	-0.1696627060
H19	3.6167147768	2.5033443049	0.2176412065
H20	0.9686918089	3.2163809645	0.4691984015

#####mol\_reduced#####

20

structure

C1	-3.3886921466	0.0896697692	0.1885821774
C2	-2.9157873703	1.3987484944	0.3757648233
N3	-1.6293900482	1.7281085819	0.3628009560

C4	-0.7285872984	0.7417261113	0.1572047750
C5	-1.0954348725	-0.6260919792	-0.0447666113
C6	-2.4661940336	-0.9202425296	-0.0219207471
C7	0.6709084758	1.0450652118	0.1341155732
C8	1.5974709261	0.0346448559	-0.0764630148
C9	1.3410979491	-1.3743686819	-0.2905622083
C10	-0.1182068721	-1.7158186618	-0.2708626703
O11	2.8665291817	0.5610711998	-0.0568334776
C12	2.7257606694	1.9038949768	0.1668595732
C13	1.4208239499	2.2568597201	0.2908745919
O14	-0.5082077270	-2.8888242611	-0.4402754377
O15	2.2392000007	-2.2162878537	-0.4723340450
H16	-4.4548049320	-0.1129789826	0.2106563609
H17	-3.6176391410	2.2148733850	0.5437049172
H18	-2.7559160449	-1.9541898544	-0.1740747409
H19	3.6457969331	2.4640943864	0.2098267062
H20	1.0231246770	3.2429706785	0.4703005527

#####mol\_double\_reduced#####

20

structure

C1	-3.3919278967	0.0779216123	0.1869803683
C2	-2.9318269287	1.4094134133	0.3782772101
N3	-1.6517565345	1.7525371473	0.3677677656
C4	-0.7215032116	0.7802601697	0.1629731136
C5	-1.0718208068	-0.6298802800	-0.0466578756
C6	-2.4528302262	-0.9150123730	-0.0216633201
C7	0.6541741298	1.0695990729	0.1388951819
C8	1.5726591862	0.0146726422	-0.0783733239
C9	1.3344147667	-1.3788345112	-0.2909524298
C10	-0.1193602559	-1.7178310639	-0.2712272529
O11	2.8767452015	0.5487291165	-0.0592255973
C12	2.7378207952	1.8976265596	0.1653226403
C13	1.4357480234	2.2638688692	0.2912530181
O14	-0.5211231525	-2.9119419839	-0.4435148008
O15	2.2570943055	-2.2296054176	-0.4753029005
H16	-4.4599061304	-0.1398182875	0.2068137960
H17	-3.6509982586	2.2180372579	0.5458432417
H18	-2.7239572208	-1.9568810545	-0.1759413757
H19	3.6613964763	2.4588426892	0.2083221865
H20	1.0552044738	3.2602144609	0.4714052796

#####mol110#####

#####mol#####

20

structure

C1	-3.4105398745	0.2078231525	0.1754745958
C2	-2.8574571142	1.4793159317	0.3284681514
N3	-1.5462121814	1.7278047343	0.3067317904
C4	-0.7167574325	0.6923851253	0.1273296804
C5	-1.1749784682	-0.6307016520	-0.0367291910

C6	-2.5488315672	-0.8646717697	-0.0103932953
C7	0.7243678413	0.9661265522	0.1032001090
C8	1.6453459179	-0.0522494858	-0.0783241561
C9	1.3048497377	-1.4550912873	-0.2585361055
C10	-0.2279597199	-1.7665411072	-0.2349104888
S11	3.2763575502	0.5468193205	-0.0658993399
C12	2.7034942973	2.1574534803	0.1829983195
C13	1.3388857379	2.2369157277	0.2532796628
O14	-0.6018159175	-2.9065590000	-0.3761899959
O15	2.1034621762	-2.3520806773	-0.4180395859
H16	-4.4843424164	0.0707049237	0.2023978859
H17	-3.4992823608	2.3432167846	0.4760245357
H18	-2.9092489412	-1.8787438384	-0.1358351626
H19	3.4156533346	2.9650137644	0.2644367312
H20	0.7806353121	3.1490016042	0.4043566946

#####mol\_reduced#####

20

structure

C1	-3.3956774479	0.1897742176	0.1727465667
C2	-2.8667137866	1.4815879356	0.3293590796
N3	-1.5687493601	1.7546849210	0.3111208460
C4	-0.7048467145	0.7286725230	0.1313449393
C5	-1.1332738902	-0.6227867716	-0.0378738799
C6	-2.5153658756	-0.8607560245	-0.0112935486
C7	0.7082111074	0.9980786055	0.1078562045
C8	1.5971824971	-0.0606167791	-0.0771111071
C9	1.2633687135	-1.4568604648	-0.2566624366
C10	-0.2036732574	-1.7558602871	-0.2353081923
S11	3.2596917660	0.5029236411	-0.0701083861
C12	2.7248515528	2.1521363083	0.1814916402
C13	1.3691701672	2.2569463025	0.2540203558
O14	-0.6335835733	-2.9155325280	-0.3780183703
O15	2.1326819843	-2.3357486850	-0.4159264972
H16	-4.4692781025	0.0330114703	0.1974541931
H17	-3.5329283295	2.3308870545	0.4761885485
H18	-2.8467955488	-1.8853496100	-0.1393921475
H19	3.4563876222	2.9429489618	0.2598411230
H20	0.8303953620	3.1827686540	0.4053916623

#####mol\_double\_reduced#####

20

structure

C1	-3.4019042333	0.1792350147	0.1723262892
C2	-2.8852172936	1.4916519976	0.3315342577
N3	-1.5952911140	1.7824906892	0.3152514591
C4	-0.6983219923	0.7692977711	0.1357722559
C5	-1.1132713295	-0.6209187435	-0.0391648631
C6	-2.5020694656	-0.8541616232	-0.0106796034
C7	0.6886587294	1.0267505200	0.1119732238
C8	1.5640590294	-0.0793031119	-0.0781904848

C9	1.2581309860	-1.4559305955	-0.2564226728
C10	-0.2038729240	-1.7535578971	-0.2359184891
S11	3.2699648518	0.4747829256	-0.0730172082
C12	2.7420292475	2.1533722477	0.1817693346
C13	1.3860026356	2.2654303893	0.2537548204
O14	-0.6474338292	-2.9300312098	-0.3807338589
O15	2.1535462817	-2.3426487930	-0.4171373184
H16	-4.4773213260	0.0070434922	0.1960163323
H17	-3.5701742984	2.3329874600	0.4782711231
H18	-2.8138034425	-1.8876391316	-0.1404057295
H19	3.4780663728	2.9433282660	0.2603446349
H20	0.8598512328	3.2026105819	0.4050063948

#####mol111#####

#####mol#####

15

structure

C1	-1.3200465054	2.0382828555	0.1067144157
C2	-0.1289145086	1.1864727658	0.0943001923
C3	-0.1312274250	-0.1837402744	0.0935274493
C4	-1.3981495135	-0.9370530550	0.1057555446
C5	-2.6305377136	-0.0888137788	0.1185774894
C6	-2.5935991206	1.2515267503	0.1189946934
C7	1.2359094559	-0.5905860024	0.0796236266
C8	1.9539204325	0.5665468470	0.0731277514
O9	1.1373077938	1.6584205383	0.0819167660
O10	-1.4600521888	-2.1517094122	0.1056584568
O11	-1.3068795916	3.2537732695	0.1072942116
H12	-3.5653600488	-0.6384288028	0.1275983574
H13	-3.4970235359	1.8512085062	0.1283769162
H14	1.6196445598	-1.5974707292	0.0751936390
H15	3.0096661397	0.7787248667	0.0627054048

#####mol\_reduced#####

15

structure

C1	-1.3316232232	2.0542436062	0.1068362532
C2	-0.1616257794	1.2014794217	0.0946343342
C3	-0.1679563369	-0.1837847735	0.0938844365
C4	-1.4044717631	-0.9543844730	0.1058063204
C5	-2.5866196549	-0.1164816969	0.1181247167
C6	-2.5478064934	1.2622650443	0.1185427242
C7	1.2097125558	-0.5862410092	0.0798816615
C8	1.9366035911	0.5596459483	0.0732985294
O9	1.1322874166	1.6677659742	0.0819869198
O10	-1.4298266425	-2.2111051457	0.1053281216
O11	-1.3013618191	3.3106086972	0.1072659732
H12	-3.5385493560	-0.6415227842	0.1273336136
H13	-3.4701751639	1.8377705527	0.1280997195
H14	1.5815450831	-1.5990849474	0.0755684141
H15	2.9963843678	0.7593654067	0.0628323738



#####mol\_double\_reduced#####

15

structure

C1	-1.3360405325	2.0899067106	0.1069025304
C2	-0.1941788327	1.2229018528	0.0949758285
C3	-0.1988422146	-0.1891040088	0.0941955287
C4	-1.4067151811	-0.9912428598	0.1058091200
C5	-2.5560156186	-0.1475916099	0.1177893813
C6	-2.5129843649	1.2716929016	0.1181904844
C7	1.1815246288	-0.5831230504	0.0801662993
C8	1.9263095563	0.5543415919	0.0733934389
O9	1.1382711488	1.6796466207	0.0819319412
O10	-1.3999125365	-2.2838270142	0.1049919760
O11	-1.3036591333	3.3813651078	0.1073380884
H12	-3.5270687047	-0.6520872700	0.1272060449
H13	-3.4555102591	1.8281874470	0.1279407355
H14	1.5385034595	-1.6052125534	0.0759951314
H15	2.9938603483	0.7349709809	0.0628300312

#####mol112#####

#####mol#####

15

structure

C1	-1.4504052710	2.0666950298	0.1090592763
C2	-0.1934400096	1.3079146309	0.0952851902
C3	-0.1269041743	-0.0704463020	0.0932054272
C4	-1.3667137036	-0.8801473970	0.1050818078
C5	-2.6453433618	-0.1132536653	0.1190356885
C6	-2.6833885623	1.2258279520	0.1208562000
C7	1.2051628274	-0.5615632457	0.0790656211
C8	2.1189545918	0.4555397545	0.0707396616
S9	1.3815616479	2.0230588174	0.0797487875
O10	-1.3583622424	-2.0977437525	0.1036966359
O11	-1.5063774832	3.2837370439	0.1109537064
H12	-3.5452170219	-0.7185157333	0.1276311363
H13	-3.6157257724	1.7795305443	0.1310318657
H14	1.4546862331	-1.6130712354	0.0754540844
H15	3.1957658122	0.3792834489	0.0596933375

#####mol\_reduced#####

15

structure

C1	-1.4586567820	2.0797215020	0.1090867528
C2	-0.2322101318	1.3111333822	0.0957116163
C3	-0.1591183180	-0.0798898220	0.0935096116
C4	-1.3698765665	-0.9010768078	0.1050779149
C5	-2.5996831408	-0.1353911038	0.1185151488
C6	-2.6395843127	1.2388763491	0.1203563757
C7	1.1897921857	-0.5555016473	0.0791662400
C8	2.1086331217	0.4481331204	0.0707933966
S9	1.3668994540	2.0360429606	0.0801025836

O10	-1.3339402373	-2.1568970819	0.1033863957
O11	-1.4886592456	3.3369342830	0.1106769926
H12	-3.5174010068	-0.7182131792	0.1273356215
H13	-3.5897300397	1.7672826096	0.1306693989
H14	1.4289460449	-1.6113490195	0.0755916528
H15	3.1858189146	0.3645802878	0.0596367451

#####mol\_double\_reduced#####

15

structure

C1	-1.4581972722	2.1081929009	0.1091498705
C2	-0.2698144363	1.3250311506	0.0961143104
C3	-0.1858861916	-0.0942703342	0.0937786167
C4	-1.3679865834	-0.9409616285	0.1050298720
C5	-2.5689833389	-0.1625873275	0.1181800392
C6	-2.6051892116	1.2444472702	0.1200298492
C7	1.1674901523	-0.5493356690	0.0794215122
C8	2.1055946251	0.4404464395	0.0708350997
S9	1.3666126913	2.0546583739	0.0800312038
O10	-1.3154828808	-2.2274027639	0.1031408272
O11	-1.4892894431	3.3993252086	0.1108145463
H12	-3.5052463929	-0.7269508772	0.1271923051
H13	-3.5720536919	1.7558598947	0.1304914207
H14	1.3919530585	-1.6124774375	0.0760027876
H15	3.1842931794	0.3413450970	0.0596902717

#####mol113#####

#####mol#####

15

structure

C1	-1.3751293323	2.0824677388	0.1074757973
C2	-0.1299688002	1.3012946977	0.0930056873
C3	-0.1291077296	-0.1361613072	0.0916086626
C4	-1.3733406039	-0.9188514124	0.1045551793
C5	-2.6154957839	-0.0909044289	0.1190335583
C6	-2.6162944948	1.2530159931	0.1203440717
C7	1.1769936914	-0.5164336951	0.0768584262
O8	1.9769377923	0.5838595535	0.0691018977
C9	1.1756645837	1.6831678631	0.0789897205
O10	-1.4174155879	-2.1357426456	0.1038622886
O11	-1.4206512600	3.2993031233	0.1091491700
H12	-3.5404610163	-0.6579028887	0.1286672522
H13	-3.5419331591	1.8188926310	0.1310826663
H14	1.6721890980	-1.4720107904	0.0704769636
H15	1.6696983147	2.6393583536	0.0744615224

#####mol\_reduced#####

15

structure

C1	-1.3987852372	2.0965342792	0.1077605081
C2	-0.1563717045	1.3056878586	0.0932900424
C3	-0.1555058550	-0.1405842888	0.0918878413

C4	-1.3969774166	-0.9329459932	0.1048116066
C5	-2.5779373907	-0.1165092325	0.1185748619
C6	-2.5787685506	1.2786643813	0.1199330468
C7	1.1556012573	-0.5174812950	0.0770738362
O8	1.9688477064	0.5838528138	0.0691615054
C9	1.1542744175	1.6841877177	0.0792016980
O10	-1.3875480798	-2.1891692734	0.1035282323
O11	-1.3908739011	3.3527680509	0.1089271914
H12	-3.5214274689	-0.6571009365	0.1284143866
H13	-3.5228945397	1.8181263162	0.1308231770
H14	1.6476391946	-1.4745884359	0.0707288159
H15	1.6451521122	2.6418998273	0.0747143377

#####mol\_double\_reduced#####

15

structure

C1	-1.4142622368	2.1283238001	0.1079507180
C2	-0.1875290291	1.3148003663	0.0936524690
C3	-0.1866609290	-0.1497087436	0.0922316311
C4	-1.4123839560	-0.9647360080	0.1049440904
C5	-2.5527985758	-0.1454973029	0.1182888086
C6	-2.5536737434	1.3076826746	0.1197015056
C7	1.1330168934	-0.5194903796	0.0773338891
O8	1.9620580933	0.5838192055	0.0692587095
C9	1.1317255385	1.6861420033	0.0794738495
O10	-1.3496580141	-2.2584373286	0.1030057588
O11	-1.3532204087	3.4221014840	0.1085326856
H12	-3.5167489553	-0.6643950285	0.1283946049
H13	-3.5182297339	1.8254361361	0.1308204925
H14	1.6218099507	-1.4806319177	0.0710237052
H15	1.6194017594	2.6478641299	0.0750273289

#####mol114#####

#####mol#####

15

structure

C1	-1.3682905660	2.0718324010	0.1076690461
C2	-0.1072639206	1.2989516185	0.0923472182
C3	-0.1074408681	-0.1346280980	0.0910465256
C4	-1.3686307536	-0.9072432644	0.1049557563
C5	-2.6134681606	-0.0886605388	0.1201342544
C6	-2.6133097998	1.2535066640	0.1213577986
C7	1.1538576526	-0.6627264769	0.0759773168
S8	2.3507389862	0.5818751505	0.0632987980
C9	1.1541654554	1.8267645732	0.0782317705
O10	-1.4118265092	-2.1241964529	0.1043445227
O11	-1.4112099238	3.2887926950	0.1092818187
H12	-3.5358425879	-0.6595849088	0.1303040211
H13	-3.5355521592	1.8246237780	0.1325720804
H14	1.4308805373	-1.7055734255	0.0718259202
H15	1.4314350189	2.8695510470	0.0759661103

#####mol\_reduced#####

15

structure

C1	-1.3881137312	2.0883300120	0.1079237720
C2	-0.1316495091	1.3046393693	0.0926468913
C3	-0.1318271829	-0.1403178411	0.0913340131
C4	-1.3884718260	-0.9237502909	0.1051891884
C5	-2.5708270921	-0.1135937453	0.1196217210
C6	-2.5706606566	1.2784219019	0.1208837242
C7	1.1339939758	-0.6666522329	0.0762040168
S8	2.3355958570	0.5818912578	0.0634213307
C9	1.1343031114	1.8306997807	0.0784819223
O10	-1.3805567365	-2.1793627439	0.1039684381
O11	-1.3799046251	3.3439417612	0.1089854011
H12	-3.5115827412	-0.6586685571	0.1300203097
H13	-3.5112875847	1.8236973559	0.1322695090
H14	1.4054912052	-1.7105481578	0.0721247011
H15	1.4060551679	2.8745354775	0.0763054453

#####mol\_double\_reduced#####

15

structure

C1	-1.4000893174	2.1237094002	0.1080931760
C2	-0.1615464518	1.3158493658	0.0929974586
C3	-0.1617307747	-0.1514743836	0.0916651004
C4	-1.4004213479	-0.9591051185	0.1052877981
C5	-2.5397826300	-0.1417458647	0.1192133667
C6	-2.5396141431	1.3065589112	0.1205335495
C7	1.1118339141	-0.6716647460	0.0764438116
S8	2.3256730694	0.5818599619	0.0635706559
C9	1.1121691876	1.8357155568	0.0787171652
O10	-1.3444798770	-2.2505178313	0.1034860674
O11	-1.3439938803	3.4151089658	0.1086477239
H12	-3.5020469195	-0.6619979674	0.1298752346
H13	-3.5017310940	1.8270577965	0.1321481430
H14	1.3745330402	-1.7190016567	0.0724362531
H15	1.3752155052	2.8829706163	0.0766058659

#####mol115#####

#####mol#####

15

structure

C1	-1.9467666808	1.6433132908	0.1018704114
C2	-0.7618487739	0.9222945067	0.0947718287
C3	-0.7527367715	-0.4658796981	0.0961451669
C4	-1.9280525084	-1.2024276959	0.1046733114
C5	-3.1269791218	-0.4877152811	0.1118554523
C6	-3.1361868351	0.9128906175	0.1104803085
C7	0.6627180859	-0.9110246237	0.0872423761
O8	1.4529134064	0.2426978568	0.0807843925
C9	0.6476586329	1.3859715423	0.0849628118

O10	1.1037955492	2.4858007976	0.0808261911
O11	1.1332201788	-2.0047875089	0.0852854175
H12	-1.9424489091	2.7262913229	0.1007307356
H13	-1.9094674623	-2.2852578933	0.1056649061
H14	-4.0694122640	-1.0227789822	0.1186266575
H15	-4.0855796346	1.4355120318	0.1162191240

#####mol\_reduced#####

15

structure

C1	-1.9566075516	1.6429454108	0.1019188073
C2	-0.7380539206	0.94444449412	0.0945903352
C3	-0.7286458189	-0.4877156952	0.0960012624
C4	-1.9378860000	-1.2021760506	0.1047418251
C5	-3.1295225150	-0.5035277903	0.1118987107
C6	-3.1389372285	0.9286907670	0.1104759602
C7	0.6366889065	-0.9283452448	0.0874149659
O8	1.4298337722	0.2425383790	0.0809695051
C9	0.6213609154	1.4029401835	0.0851415107
O10	1.1272870735	2.5168267939	0.0806678822
O11	1.1571612477	-2.0355179328	0.0851079665
H12	-1.9563837957	2.7290620691	0.1007754983
H13	-1.9233423941	-2.2881930367	0.1057738697
H14	-4.0735588518	-1.0402789168	0.1186986305
H15	-4.0899515782	1.4529946083	0.1162207124

#####mol\_double\_reduced#####

15

structure

C1	-1.9694138235	1.6447670083	0.1020041713
C2	-0.7241917253	0.9741737076	0.0944554147
C3	-0.7144706308	-0.5171044294	0.0959312998
C4	-1.9505704278	-1.2040811537	0.1048208009
C5	-3.1483786189	-0.5210402063	0.1120382752
C6	-3.1579761166	0.9459149007	0.1105892528
C7	0.6175405528	-0.9514065093	0.0875774525
O8	1.4105210284	0.2422869818	0.0811018609
C9	0.6018972698	1.4258190732	0.0852321963
O10	1.1672398216	2.5488711671	0.0803534061
O11	1.1972763300	-2.0671172181	0.0849053252
H12	-1.9771180013	2.7376333251	0.1009273538
H13	-1.9436981171	-2.2969544078	0.1059020629
H14	-4.0946618502	-1.0645475580	0.1188540647
H15	-4.1113532549	1.4769289662	0.1163492142

#####mol116#####

#####mol#####

15

structure

C1	-1.9306114670	1.6325949418	0.1029770567
C2	-0.7342507363	0.9246668905	0.0947719146
C3	-0.7260588611	-0.4686324728	0.0952824921

C4	-1.9140077474	-1.1905826977	0.1039964192
C5	-3.1169397642	-0.4850162927	0.1122416158
C6	-3.1251572465	0.9129222609	0.1117392417
C7	0.6308357205	-1.0807208970	0.0859219111
S8	1.8952639644	0.2434665343	0.0764468542
C9	0.6153611244	1.5526757597	0.0849301660
O10	0.8616127281	2.7247708948	0.0826710919
O11	0.8908730746	-2.2498336422	0.0845590775
H12	-1.9189805011	2.7155872467	0.1024581442
H13	-1.8896284247	-2.2733625014	0.1042633226
H14	-4.0561716329	-1.0257286789	0.1191245724
H15	-4.0706824338	1.4425577673	0.1182360037

#####mol\_reduced#####

15

structure

C1	-1.9319881770	1.6312381632	0.1029587696
C2	-0.6988440379	0.9453749761	0.0944814252
C3	-0.6904262254	-0.4886878093	0.0950102759
C4	-1.9152710465	-1.1891289625	0.1040068516
C5	-3.1088809345	-0.4995188856	0.1122050763
C6	-3.1173445541	0.9274535397	0.1116710294
C7	0.6038318067	-1.1130731746	0.0861161801
S8	1.8682161859	0.2432139504	0.0765731461
C9	0.5881511306	1.5847678016	0.0851340755
O10	0.8770484470	2.7780103067	0.0826682244
O11	0.9063039126	-2.3029527500	0.0845184593
H12	-1.9196236462	2.7164065961	0.1024323740
H13	-1.8899079203	-2.2740706650	0.1042907252
H14	-4.0503815434	-1.0408496115	0.1191405551
H15	-4.0652482208	1.4575015326	0.1182018581

#####mol\_double\_reduced#####

15

structure

C1	-1.9392592167	1.6319957803	0.1030074408
C2	-0.6737212018	0.9745478186	0.0942849574
C3	-0.6649535499	-0.5177809063	0.0948323053
C4	-1.9226452671	-1.1900690511	0.1040387642
C5	-3.1181572992	-0.5156984633	0.1122709140
C6	-3.1267400930	0.9436030755	0.1117402697
C7	0.5763210922	-1.1631212971	0.0863459879
S8	1.8628010323	0.2432444211	0.0766363648
C9	0.5598599051	1.6344562771	0.0853048881
O10	0.8977501786	2.8418280643	0.0824573792
O11	0.9283371074	-2.3664539606	0.0844013039
H12	-1.9315259238	2.7221328435	0.1025146841
H13	-1.9020608831	-2.2800405099	0.1043452413
H14	-4.0621866370	-1.0623153962	0.1192262815
H15	-4.0771389530	1.4790835384	0.1182997816

#####mol117#####

#####mol#####

15

structure

C1	-0.8596588648	2.4901065215	0.1023058511
C2	0.2256620788	1.7003579538	0.0944662153
C3	0.2205065581	0.2292435637	0.0958556609
C4	-0.9351597945	-0.4751822910	0.1056613096
C5	-2.2108855214	0.2489299276	0.1150876013
C6	-2.1714374643	1.8283237908	0.1132969859
C7	1.6217034744	-0.1367154110	0.0851061295
C8	2.3180244336	1.0129976705	0.0785939747
O9	1.5252404646	2.1404819170	0.0838186960
O10	-3.2876311356	-0.3077194071	0.1241398564
O11	-3.2159980542	2.4407511915	0.1209976378
H12	-0.8129471880	3.5710670058	0.1009328421
H13	-0.9679873160	-1.5578516222	0.1069351430
H14	2.0327228112	-1.1329553025	0.0827534660
H15	3.3778946341	1.2124391888	0.0700693224

#####mol\_reduced#####

15

structure

C1	-0.8801173520	2.4507932718	0.1025205324
C2	0.2450997987	1.6727183119	0.0943432327
C3	0.2433335124	0.2450833509	0.0956828553
C4	-0.9634278140	-0.4390585700	0.1058512129
C5	-2.2177023953	0.2661367772	0.1151126889
C6	-2.1782981449	1.8086240842	0.1133860559
C7	1.6371684346	-0.1287371568	0.0850136020
C8	2.3572527572	1.0196046673	0.0782590984
O9	1.5517352504	2.1389533870	0.0835804765
O10	-3.3180802260	-0.3220897064	0.1243466681
O11	-3.2369858495	2.4584811725	0.1211746374
H12	-0.8395487110	3.5342355426	0.1011883678
H13	-1.0069936728	-1.5244791798	0.1071917581
H14	2.0434333140	-1.1297290479	0.0827286264
H15	3.4172139053	1.2181042034	0.0697057226

#####mol\_double\_reduced#####

15

structure

C1	-0.8921374205	2.4285485376	0.1026550468
C2	0.2716796891	1.6564800401	0.0941634227
C3	0.2678630905	0.2514242107	0.0955012608
C4	-0.9898698213	-0.4260574976	0.1060591582
C5	-2.2351489592	0.2567831409	0.1152535192
C6	-2.1850492174	1.8031462018	0.1134476259
C7	1.6502713179	-0.1204146179	0.0849212799
C8	2.4088548423	1.0290214117	0.0778242613
O9	1.5778937711	2.1415694262	0.0833700010
O10	-3.3646749135	-0.3283663553	0.1246857580

O11	-3.2574473509	2.4741629756	0.1213103298
H12	-0.8568932419	3.5181695823	0.1013719552
H13	-1.0323794391	-1.5183176584	0.1073969945
H14	2.0499893966	-1.1302557266	0.0827078912
H15	3.4695595920	1.2310374929	0.0692353149

#####mol118#####

#####mol#####

15

structure

C1	-0.9930226398	2.5130480828	0.1038126269
C2	0.1603586037	1.8158244901	0.0945963208
C3	0.2242081003	0.3354610988	0.0954659824
C4	-0.9058414793	-0.4142485699	0.1059068054
C5	-2.2243663355	0.2226684796	0.1166309282
C6	-2.2725163922	1.7906231812	0.1154759809
C7	1.5987584136	-0.1183265826	0.0840888403
C8	2.4942141133	0.8850452466	0.0754564869
S9	1.7938027978	2.5063237214	0.0799340968
O10	-3.2628311075	-0.4039309892	0.1262090850
O11	-3.3437118012	2.3566947115	0.1240732135
H12	-1.0354475963	3.5955215121	0.1031264758
H13	-0.8778515511	-1.4978424172	0.1067191132
H14	1.8711608997	-1.1649314549	0.0827356219
H15	3.5711708483	0.7954194497	0.0662977388

#####mol\_reduced#####

15

structure

C1	-1.0162408483	2.4799513361	0.1040284132
C2	0.1736395775	1.7963812920	0.0945215941
C3	0.2440437079	0.3601090061	0.0952800713
C4	-0.9334916286	-0.3764957327	0.1061148420
C5	-2.2313130274	0.2405754022	0.1166637473
C6	-2.2803570912	1.7725989519	0.1155207834
C7	1.6075372576	-0.1027470624	0.0839716827
C8	2.5358815151	0.8848012562	0.0750716103
S9	1.8135769422	2.4972473016	0.0798590622
O10	-3.2894164630	-0.4203020193	0.1264408628
O11	-3.3685525989	2.3719589085	0.1241868389
H12	-1.0648028878	3.5641604970	0.1033631625
H13	-0.9100548733	-1.4632039166	0.1069787558
H14	1.8679411373	-1.1553491690	0.0826793470
H15	3.6115914684	0.7894530999	0.0658666621

#####mol\_double\_reduced#####

15

structure

C1	-1.0317830374	2.4622778816	0.1041920406
C2	0.1913645594	1.7882172619	0.0943899845
C3	0.2651517168	0.3725898797	0.0951031976
C4	-0.9605884728	-0.3617844547	0.1063467360



C5	-2.2490514104	0.2307323966	0.1168176226
C6	-2.2902458476	1.7665857851	0.1156190342
C7	1.6142888394	-0.0860281443	0.0839076808
C8	2.5890897942	0.8876050811	0.0745983961
S9	1.8371610268	2.4936519560	0.0796603180
O10	-3.3347651189	-0.4283151076	0.1267942049
O11	-3.3923348156	2.3833203980	0.1243826929
H12	-1.0851327991	3.5513319753	0.1035624553
H13	-0.9298888522	-1.4545629835	0.1071606342
H14	1.8642824749	-1.1466472706	0.0827284114
H15	3.6647313502	0.7860683549	0.0653833811

#####mol119#####

#####mol#####

15

structure

C1	-0.6749203457	1.9624747662	0.0996028897
C2	0.4814275986	1.0838955624	0.0913481281
C3	0.4278326036	-0.2911083934	0.0962421589
C4	-0.8453335591	-0.9955680592	0.1106442352
C5	-2.0038423770	-0.3110662960	0.1196004668
C6	-2.0387635564	1.1708435073	0.1153109326
C7	1.7831506763	-0.7370183954	0.0847237780
C8	2.5434076472	0.3968504645	0.0738527585
O9	1.7714418860	1.5097575019	0.0776667617
O10	-0.6583075134	3.1714168943	0.0955001457
O11	-3.0749309211	1.7944268167	0.1234247607
H12	-0.8412370087	-2.0801878068	0.1140044050
H13	-2.9677981235	-0.8054041429	0.1303816042
H14	2.1481318704	-1.7517549549	0.0844789838
H15	3.6072167821	0.5662579523	0.0631656780

#####mol\_reduced#####

15

structure

C1	-0.7006942256	1.9388726800	0.0999794839
C2	0.4430809559	1.0634693418	0.0918104849
C3	0.4247205837	-0.3303280554	0.0964194272
C4	-0.8227147875	-1.0150868502	0.1105313351
C5	-1.9769787424	-0.2704617482	0.1192252569
C6	-2.0164834092	1.1861827609	0.1149945294
C7	1.8035504343	-0.7392386260	0.0845184773
C8	2.5401268491	0.4031889126	0.0738328488
O9	1.7501862933	1.5147792531	0.0778629482
O10	-0.6286488600	3.1827248761	0.0953243664
O11	-3.1024370077	1.8065122136	0.1234544583
H12	-0.8523326660	-2.1011896445	0.1142478585
H13	-2.9513907846	-0.7517759400	0.1300752014
H14	2.1925297421	-1.7475603352	0.0840005903
H15	3.6029155290	0.5869462699	0.0630726151

#####mol\_double\_reduced#####

15

structure

C1	-0.7043177980	1.9382175382	0.1000126258
C2	0.4103689065	1.0597063602	0.0921321097
C3	0.4238853510	-0.3678859533	0.0965408038
C4	-0.7987642478	-1.0448303790	0.1103950233
C5	-1.9654976892	-0.2527549373	0.1190532227
C6	-2.0198019051	1.1885390552	0.1150151629
C7	1.8131033629	-0.7452281435	0.0844431968
C8	2.5471264330	0.4027095388	0.0737730873
O9	1.7633806518	1.5229595460	0.0777231640
O10	-0.6248217191	3.2096890472	0.0952043718
O11	-3.1311178854	1.8170278522	0.1236963480
H12	-0.8485452702	-2.1358164607	0.1143326668
H13	-2.9489817197	-0.7327496274	0.1299953771
H14	2.2205054913	-1.7523531142	0.0837399439
H15	3.6169200345	0.5747690106	0.0629765007

#####mol120#####

#####mol#####

15

structure

C1	-0.8043370105	1.9881008454	0.1027943038
C2	0.4207001054	1.1972735270	0.0921920031
C3	0.4366350655	-0.1886874908	0.0951761077
C4	-0.8106380668	-0.9424680491	0.1094015120
C5	-2.0090284700	-0.3301424974	0.1200988963
C6	-2.1285758743	1.1413473213	0.1180502879
C7	1.7586762166	-0.7109328463	0.0830809121
C8	2.7065832557	0.2785114798	0.0712999803
S9	2.0216450323	1.8622883341	0.0745136448
O10	-0.8498674313	3.1982457481	0.1005609249
O11	-3.1941879311	1.7141739244	0.1275360819
H12	-0.7482539142	-2.0260455623	0.1111682094
H13	-2.9406295060	-0.8833407367	0.1306827404
H14	1.9960641649	-1.7665505122	0.0831053792
H15	3.7800147238	0.1639339807	0.0608013615

#####mol\_reduced#####

15

structure

C1	-0.8220457887	1.9635221747	0.1030126247
C2	0.3796905940	1.1702960639	0.0926626584
C3	0.4359965544	-0.2303489525	0.0952554675
C4	-0.7868745466	-0.9638075142	0.1091887326
C5	-1.9832370642	-0.2936144173	0.1197670241
C6	-2.1046244442	1.1564782159	0.1177955751
C7	1.7844043004	-0.7145157338	0.0828211654
C8	2.7154110915	0.2803549168	0.0712392669
S9	1.9930217579	1.8753958071	0.0747632159
O10	-0.8109854638	3.2102349970	0.1000933807

O11	-3.2162976250	1.7220074114	0.1278090985
H12	-0.7566865317	-2.0505756780	0.1112915967
H13	-2.9260975750	-0.8339380260	0.1304564022
H14	2.0409094808	-1.7688036866	0.0826379236
H15	3.7909941050	0.1805221778	0.0607268262

#####mol\_double\_reduced#####

15

structure

C1	-0.8227767600	1.9601588144	0.1029882948
C2	0.3419077982	1.1615388432	0.0931032832
C3	0.4356096151	-0.2692092585	0.0953517048
C4	-0.7649012159	-0.9924666571	0.1090556834
C5	-1.9732428303	-0.2814642131	0.1196263546
C6	-2.1059021178	1.1556627224	0.1177199498
C7	1.7918619836	-0.7205900333	0.0826921613
C8	2.7297039379	0.2725622145	0.0710546598
S9	1.9957908084	1.8939914584	0.0749048877
O10	-0.8045783605	3.2341119170	0.0999104486
O11	-3.2408799653	1.7254558333	0.1278574407
H12	-0.7523714891	-2.0845920392	0.1113843596
H13	-2.9248071356	-0.8198014634	0.1304131698
H14	2.0580611906	-1.7788653409	0.0823380164
H15	3.8076311677	0.1652770799	0.0604099284

#####mol121#####

#####mol#####

15

structure

C1	-0.7521390132	2.0131990295	0.1063409850
C2	0.4852625584	1.2328721440	0.0959061907
C3	0.4291287523	-0.1397221892	0.0942997606
C4	-0.7610751040	-0.9460283616	0.1020599682
C5	-1.9601354673	-0.3274528186	0.1119968667
C6	-2.0752582303	1.1497543087	0.1150471063
O7	1.6756493114	-0.6624834717	0.0841650147
C8	2.5449840398	0.3998411499	0.0792023791
C9	1.8723346921	1.5802663975	0.0860055752
O10	-0.8156770346	3.2200350272	0.1085524003
O11	-3.1452442475	1.7142702663	0.1239465734
H12	-0.6661900968	-2.0257828277	0.0997498898
H13	-2.8929433461	-0.8775621013	0.1182032122
H14	3.5896296975	0.1407015373	0.0709685007
H15	2.2963271861	2.5709772551	0.0842887031

#####mol\_reduced#####

15

structure

C1	-0.7765029469	1.9906169241	0.1064759440
C2	0.4412860059	1.2002452887	0.0961756553
C3	0.4267361689	-0.1899175852	0.0942370494
C4	-0.7434473377	-0.9677032249	0.1018820911

C5	-1.9396514373	-0.2725125621	0.1119214380
C6	-2.0558906616	1.1743623970	0.1149487313
O7	1.7144095287	-0.6839550700	0.0838450194
C8	2.5421563959	0.4206204613	0.0792678794
C9	1.8290465719	1.5734356651	0.0863126068
O10	-0.7737652770	3.2344999442	0.1082352754
O11	-3.1755107004	1.7391922582	0.1242572613
H12	-0.6972286591	-2.0512618382	0.0999241078
H13	-2.8856038556	-0.8068905349	0.1182487345
H14	3.5978332308	0.2022634165	0.0710326837
H15	2.2187526048	2.5797524867	0.0848685149

#####mol\_double\_reduced#####

15

structure

C1	-0.7816695217	1.9809624322	0.1065230140
C2	0.4155651248	1.1800414440	0.0963463261
C3	0.4276204182	-0.2433293313	0.0941620931
C4	-0.7235112466	-0.9891544279	0.1017166353
C5	-1.9451127836	-0.2354118360	0.1120060664
C6	-2.0750919364	1.1881329323	0.1150932875
O7	1.7635318183	-0.7129636080	0.0834351471
C8	2.5551613277	0.4335545731	0.0791740205
C9	1.7993161362	1.5633630758	0.0865085872
O10	-0.7480732247	3.2509690001	0.1081242891
O11	-3.2079954995	1.7861053298	0.1245158259
H12	-0.7145838950	-2.0788823691	0.1000495692
H13	-2.8960580388	-0.7756156594	0.1183434776
H14	3.6226782915	0.2560102317	0.0708964118
H15	2.1625851346	2.5839288727	0.0852725166

#####mol122#####

#####mol#####

15

structure

C1	-0.7153895994	1.9445349058	0.1068461920
C2	0.4936721202	1.1041664924	0.0954313949
C3	0.3753274996	-0.2742592225	0.0939446831
C4	-0.8890566563	-0.9766840605	0.1030623344
C5	-2.0527875905	-0.2948205602	0.1138737721
C6	-2.0859155270	1.1796907456	0.1168399197
S7	1.9360862900	-1.0289663853	0.0798155877
C8	2.7320418395	0.5151840926	0.0760515971
C9	1.8441549435	1.5509419019	0.0851654373
O10	-0.6956316874	3.1540453396	0.1087678236
O11	-3.1181544594	1.8127396532	0.1265737363
H12	-0.8858413072	-2.0614772056	0.1010697619
H13	-3.0120121788	-0.7982245305	0.1208492763
H14	3.8102715713	0.5547857714	0.0672968401
H15	2.1228309346	2.5952678315	0.0847421256

#####mol\_reduced#####

15

structure

C1	-0.7391162443	1.9280899917	0.1070536835
C2	0.4479212990	1.0782169700	0.0957799313
C3	0.3587995862	-0.3195256099	0.0940200586
C4	-0.8792098140	-0.9968247320	0.1029545748
C5	-2.0355453377	-0.2440965523	0.1138053187
C6	-2.0685278962	1.2041903042	0.1166958096
S7	1.9697329762	-1.0474879674	0.0795368115
C8	2.7245389578	0.5431252293	0.0761227547
C9	1.8018046664	1.5398921735	0.0854727705
O10	-0.6589091992	3.1691422177	0.1086097495
O11	-3.1461719083	1.8394672631	0.1267087948
H12	-0.9185661779	-2.0817496972	0.1013136975
H13	-3.0075605195	-0.7301105546	0.1209023508
H14	3.8016936318	0.6174361604	0.0673818935
H15	2.0421926010	2.5953432275	0.0853585811

#####mol\_double\_reduced#####

15

structure

C1	-0.7466643128	1.9251336904	0.1071270207
C2	0.4219579664	1.0668480640	0.0959831616
C3	0.3446526939	-0.3688934966	0.0940581153
C4	-0.8685432284	-1.0125122314	0.1028136896
C5	-2.0453600842	-0.2062275151	0.1139073008
C6	-2.0896957751	1.2199777027	0.1168759826
S7	2.0152441344	-1.0767764133	0.0791825829
C8	2.7363818871	0.5651142910	0.0760242716
C9	1.7695278340	1.5260671914	0.0856743016
O10	-0.6490568754	3.1872508380	0.1085865166
O11	-3.1748644588	1.8887940227	0.1269850427
H12	-0.9442585837	-2.1003768870	0.1014483848
H13	-3.0222683841	-0.6968742465	0.1209937858
H14	3.8128658183	0.6739754781	0.0672947882
H15	1.9793022011	2.5921729177	0.0857862934

#####mol123#####

#####mol#####

12

structure

C1	0.7495224721	1.3841502717	0.1083645793
C2	2.2122266817	1.1429602136	0.1231743958
O3	2.9453323795	2.2803422909	0.1029981773
O4	2.7053262906	0.0423556111	0.1505196305
C5	0.1930603139	2.5972100361	0.0780680202
C6	-1.2696560442	2.8383596126	0.0632534720
O7	-2.0027236113	1.7009520685	0.0834489585
O8	-1.7627840737	3.9389482908	0.0358870743
H9	0.1467881248	0.4851667617	0.1242158826
H10	3.8750238777	2.0094917446	0.1149771921

H11	0.7957461426	3.4962289771	0.0622166000
H12	-2.9324248599	1.9717644073	0.0714561833

#####mol\_reduced#####

12

structure

C1	0.7847775197	1.3639593428	0.1090235826
C2	2.1826124285	1.1372243944	0.1231091684
O3	2.9684330617	2.3000416948	0.1026912019
O4	2.7771309162	0.0493816397	0.1508728133
C5	0.1578181385	2.6174206372	0.0774104449
C6	-1.2400422809	2.8440861207	0.0633190807
O7	-2.0258266027	1.6812557754	0.0837501698
O8	-1.8345945748	3.9319088049	0.0355386392
H9	0.1815137760	0.4650009693	0.1248284670
H10	3.8623456118	1.9364440709	0.1164855359
H11	0.7610076861	3.5164259362	0.0615993002
H12	-2.9197513239	2.0448217503	0.0699471409

#####mol\_double\_reduced#####

12

structure

C1	0.8281538082	1.3457141718	0.1097158666
C2	2.1816100405	1.1221598462	0.1234424259
O3	3.0299840690	2.3174274595	0.1027221256
O4	2.8766152853	0.0446174737	0.1516218833
C5	0.1144132381	2.6356407812	0.0767274875
C6	-1.2390729985	2.8591497849	0.0629907980
O7	-2.0873157322	1.6638782287	0.0837008783
O8	-1.9341313349	3.9367035857	0.0347980806
H9	0.2241503531	0.4413363684	0.1256444587
H10	3.8767006715	1.8533468134	0.1183662342
H11	0.7188630378	3.5396975443	0.0608192060
H12	-2.9340140130	2.1280042143	0.0680166904

#####mol124#####

#####mol#####

16

structure

C1	1.1919396139	3.3025422916	0.0887379133
C2	-0.2454293582	3.1395901347	0.0988193470
C3	2.0507379416	2.2688699377	0.1044158520
C4	3.5194661738	2.4036503925	0.0930936455
O5	3.9446889338	3.6926877443	0.0699139026
O6	4.2823502267	1.4674137130	0.1028378769
C7	-1.1041476089	4.1733606768	0.0831417798
C8	-2.5729267084	4.0388665232	0.0944243540
O9	-2.9986335804	2.7500785419	0.1169988928
O10	-3.3354657196	4.9754336252	0.0851592175
H11	1.5851273639	4.3142403192	0.0667669881
H12	-0.6386117883	2.1278940519	0.1207714728
H13	1.7032675066	1.2422095775	0.1262738409

H14	-0.7566129689	5.2000071264	0.0613020296
H15	4.9119727363	3.6591596637	0.0636572161
H16	-3.9659395132	2.7837931543	0.1233039634

#####mol\_reduced#####

16

structure

C1	1.1684878980	3.2913962810	0.0890115782
C2	-0.2221291614	3.1484252009	0.0982907696
C3	2.0931451917	2.2459862634	0.1029294361
C4	3.5078997244	2.3891319201	0.0935512314
O5	3.9608381559	3.7099623024	0.0696183263
O6	4.3527040166	1.4902899384	0.1035424181
C7	-1.1460740389	4.1944879879	0.0844489812
C8	-2.5612043585	4.0535586369	0.0939711940
O9	-3.0169105041	2.7340046021	0.1177369776
O10	-3.4040155497	4.9543741537	0.0843163660
H11	1.5684966911	4.3030752948	0.0683256747
H12	-0.6223070416	2.1368045553	0.1190125781
H13	1.7483300260	1.2172344339	0.1239407024
H14	-0.8000784501	5.2228721039	0.0632826030
H15	4.9201656808	3.6022529062	0.0643749770
H16	-3.9760427645	2.8435379268	0.1234275070

#####mol\_double\_reduced#####

16

structure

C1	1.1528138223	3.2879779912	0.0885788829
C2	-0.2061908929	3.1544761364	0.0988451851
C3	2.1498281254	2.2315020450	0.1003461596
C4	3.5253724810	2.3693112803	0.0929397266
O5	4.0180171297	3.7267855454	0.0682112093
O6	4.4466432264	1.5003000205	0.1036080069
C7	-1.2032393927	4.2109540616	0.0872402407
C8	-2.5788075398	4.0731508238	0.0945093946
O9	-3.0717933923	2.7158214214	0.1193482653
O10	-3.5000533789	4.9422807137	0.0838263986
H11	1.5556225829	4.3034410966	0.0681667278
H12	-0.6089456779	2.1389853994	0.1192893322
H13	1.8033757180	1.1987705309	0.1206649081
H14	-0.8568068972	5.2437102618	0.0668925406
H15	4.9632309101	3.5319969855	0.0682070033
H16	-4.0168950847	2.9112966248	0.1195854895

#####mol125#####

#####mol#####

20

structure

C1	4.8029727449	3.8089711741	0.1020481118
C2	3.3737942459	3.4590214484	0.1092667923
C3	2.3701866373	4.3568468305	0.0978554424
C4	0.9739696092	4.0007898561	0.1051799958

C5	-0.0294338992	4.9081160547	0.0936662893
C6	-1.4257024925	4.5522881914	0.1010301658
C7	-2.4290440719	5.4504257882	0.0896374624
O8	5.0341483515	5.1485759196	0.0824302052
C9	-3.8583853937	5.1010706107	0.0969759888
O10	5.6993773355	2.9980118630	0.1123502914
O11	-4.0901843355	3.7615773243	0.1166202364
O12	-4.7544008820	5.9124566200	0.0867561159
H13	3.1809696564	2.3923823667	0.1249499492
H14	2.6167188338	5.4144918029	0.0822029637
H15	0.7286934086	2.9411312963	0.1208671870
H16	0.2158883316	5.9677704658	0.0779720038
H17	-1.6725593158	3.4947099131	0.1167226593
H18	-2.2358672049	6.5170131707	0.0739013169
H19	5.9964009369	5.2546074054	0.0794377223
H20	-5.0524803812	3.6559345881	0.1197078628

#####mol\_reduced#####

20

structure

C1	4.8016135719	3.7948297424	0.1022478824
C2	3.4207663506	3.4341393033	0.1095628691
C3	2.3575268858	4.3278135006	0.0983163083
C4	0.9993759084	3.9948244122	0.1052593300
C5	-0.0548543696	4.9136717885	0.0936603378
C6	-1.4130879792	4.5810679197	0.1006193504
C7	-2.4759191641	5.4752616189	0.0894016337
O8	5.0428687925	5.1649764026	0.0821189222
C9	-3.8569815691	5.1153279516	0.0967522479
O10	5.7665520454	3.0323649773	0.1117733201
O11	-4.0990786597	3.7453324726	0.1168737823
O12	-4.8214481999	5.8784118680	0.0872653785
H13	3.2380425044	2.3648857800	0.1252757561
H14	2.6068493706	5.3869385923	0.0826326961
H15	0.7400534835	2.9356515752	0.1209624056
H16	0.2045475635	5.9728350324	0.0779561462
H17	-1.6629807178	3.5220816874	0.1163005766
H18	-2.2927537001	6.5444442273	0.0736915077
H19	6.0071403300	5.2150031781	0.0799321382
H20	-5.0633761103	3.6959063044	0.1190996990

#####mol\_double\_reduced#####

20

structure

C1	4.8280648767	3.7767461785	0.1024466654
C2	3.4841988086	3.4177052443	0.1097551199
C3	2.3590632173	4.3094044723	0.0986423550
C4	1.0282133380	3.9896540980	0.1053888284
C5	-0.0835425920	4.9153343947	0.0937700001
C6	-1.4146432639	4.5966662810	0.1004623236
C7	-2.5383643187	5.4902126267	0.0893427106



O8	5.0887576703	5.1840327187	0.0816832865
C9	-3.8830766824	5.1345447574	0.0964905051
O10	5.8587166070	3.0578839845	0.1112184197
O11	-4.1479980762	3.7280880228	0.1170602013
O12	-4.9117207648	5.8563305579	0.0876965908
H13	3.3042043644	2.3448477046	0.1255490039
H14	2.6090227014	5.3717285976	0.0828666823
H15	0.7618759547	2.9279247255	0.1211719905
H16	0.1835883246	5.9768480865	0.0780220276
H17	-1.6655540005	3.5345769587	0.1161751758
H18	-2.3559129594	6.5626279836	0.0736512284
H19	6.0535565248	5.1654620305	0.0804034754
H20	-5.1127363776	3.7498128381	0.1182316202

#####mol126#####

#####mol#####

16

structure

C1	1.1722922311	3.3370976053	0.0908186390
C2	-0.2538496943	3.0969059898	0.0994069686
C3	2.0993864166	2.3644282391	0.0889852354
C4	3.5547291371	2.6536221029	0.0789089261
O5	3.9742681563	3.8577152402	0.0711944159
O6	4.3673663388	1.6717453166	0.0757488105
C7	-1.1791841773	4.0712864623	0.1032882601
C8	-2.6356773650	3.7869379239	0.1130179878
O9	-3.0581858312	2.5838541775	0.1143410616
O10	-3.4448825777	4.7714146056	0.1216291553
H11	1.5199301421	4.3668389154	0.0857056479
H12	-0.6023089803	2.0674582404	0.1031412925
H13	1.8263374724	1.3145526940	0.0944110398
H14	-0.9025933054	5.1203310269	0.1003858004
Li15	5.6251691923	3.0298928023	0.0580033874
Li16	-4.7089241774	3.4201462012	0.1330800368

#####mol\_reduced#####

16

structure

C1	1.1538461013	3.3322545371	0.0933710222
C2	-0.2344733734	3.1028025391	0.1014173354
C3	2.1401774062	2.3564551825	0.0836412482
C4	3.5463853598	2.6377178213	0.0719816520
O5	4.0031975729	3.8590748086	0.0679620863
O6	4.4089061404	1.6563778700	0.0633685279
C7	-1.2171931102	4.0792951619	0.0933151933
C8	-2.6300217160	3.8015633905	0.1333017359
O9	-3.0851694027	2.5854709260	0.1551618818
O10	-3.4810458839	4.7861439229	0.1454960201
H11	1.4990927408	4.3646062157	0.0904653206
H12	-0.5818792418	2.0712578531	0.1121658930
H13	1.8703901247	1.3045439090	0.0851360573

H14	-0.9446323457	5.1306954449	0.0867993569
Li15	5.5807831669	3.0129508711	0.0388464571
Li16	-4.6832137628	3.4318058650	0.0372100298

#####mol\_double\_reduced#####

16

structure

C1	1.1743477321	3.3415167703	0.0909887363
C2	-0.2552692269	3.0977265078	0.1006595705
C3	2.1142171432	2.3807879603	0.0864187659
C4	3.5866633070	2.6589297644	0.0781196758
O5	4.0067137207	3.8539046455	0.0724642479
O6	4.3696410863	1.6607175328	0.0760583593
C7	-1.1948344906	4.0586562913	0.1053890819
C8	-2.6673410606	3.7809868134	0.1132169702
O9	-3.0874624258	2.5862045548	0.1203710929
O10	-3.4500836082	4.7793422857	0.1130933235
H11	1.5184964773	4.3734950764	0.0870273985
H12	-0.5996660897	2.0658042417	0.1045956013
H13	1.8388879313	1.3296664853	0.0903975651
H14	-0.9190915369	5.1096303170	0.1011507133
Li15	5.7840893085	3.0163658475	0.0514502753
Li16	-4.8681527382	3.4284769814	0.1411857138

#####mol127#####

#####mol#####

18

structure

C1	0.8402084835	0.2914640007	0.1047358764
C2	-0.3641710030	-0.3977224020	0.1157599753
C3	-0.3732210694	-1.7958037891	0.1063119582
C4	0.8335414302	-2.5038508618	0.0856910300
C5	2.0379198603	-1.8146625208	0.0746623466
C6	2.0469684118	-0.4165791278	0.0841168567
C7	3.3690350100	0.2711726791	0.0715574908
C8	-1.6953000068	-2.4835258730	0.1188801284
O9	3.2599432387	1.6209191779	0.0823846392
O10	4.4371119950	-0.2905879610	0.0536433412
O11	-1.5862462730	-3.8332746155	0.1081095442
O12	-2.7633562100	-1.9217232021	0.1367614946
H13	0.8538854303	1.3729310543	0.1119526734
H14	-1.3101157207	0.1283906529	0.1317162849
H15	0.8198624551	-3.5853191918	0.0784770091
H16	2.9838670513	-2.3407720927	0.0587012654
H17	4.1640816951	1.9673229194	0.0729518637
H18	-2.4903942414	-4.1796515668	0.1175574799

#####mol\_reduced#####

18

structure

C1	0.8291282624	0.2943774288	0.1049200191
C2	-0.3605939532	-0.3854368072	0.1157994805

C3	-0.4067783096	-1.8137788621	0.1066027209
C4	0.8446050653	-2.5067365936	0.0854984782
C5	2.0343358683	-1.8269217496	0.0746175450
C6	2.0805168254	-0.3985851595	0.0838229799
C7	3.3491434128	0.2663297032	0.0718115258
C8	-1.6754112355	-2.4786878049	0.1186314226
O9	3.2652250523	1.6605949102	0.0825371769
O10	4.4721750244	-0.2450180864	0.0535796770
O11	-1.5914823622	-3.8729536576	0.1079247139
O12	-2.7984401462	-1.9673414461	0.1368691041
H13	0.8351431210	1.3780628845	0.1122701374
H14	-1.3038046081	0.1494043051	0.1317895387
H15	0.8385930273	-3.5904201387	0.0781469318
H16	2.9775359068	-2.3617806712	0.0586238438
H17	4.1933344215	1.9261612011	0.0722168440
H18	-2.5195901817	-4.1385158782	0.1182611613

#####mol\_double\_reduced#####

18

structure

C1	0.8205346518	0.2987457641	0.1050916899
C2	-0.3593987188	-0.3755490637	0.1158848803
C3	-0.4438698212	-1.8349748771	0.1069589491
C4	0.8532177456	-2.5110927917	0.0853659957
C5	2.0331376504	-1.8368074367	0.0745707455
C6	2.1175915315	-0.3773631336	0.0834911091
C7	3.3472877930	0.2683657199	0.0718511334
C8	-1.6735541434	-2.4807067351	0.1185772854
O9	3.2862527450	1.7155056205	0.0825855496
O10	4.5291832743	-0.1877339326	0.0532661549
O11	-1.6125089835	-3.9278820307	0.1078627040
O12	-2.8554439258	-2.0246462799	0.1371273764
H13	0.8175044227	1.3866586452	0.1126095431
H14	-1.3009948511	0.1702882998	0.1319432870
H15	0.8561781136	-3.5989953047	0.0778576466
H16	2.9746776819	-2.3827063575	0.0585122520
H17	4.2349223115	1.8922920992	0.0714027750
H18	-2.5611729089	-4.1046993038	0.1190330038

#####mol128#####

#####mol#####

24

structure

C1	2.0487177811	-1.7847518588	0.1023202230
C2	0.8634561756	-2.5067992300	0.1023226976
C3	-0.3665278250	-1.8417194188	0.1047385852
C4	-0.4019427332	-0.4429578512	0.1071554435
C5	0.7833220417	0.2790943825	0.1071465575
C6	2.0133112444	-0.3859953487	0.1047376771
C7	3.2535985306	0.4453223531	0.1048619060
C8	-1.6067876802	-2.6730800155	0.1046187132

O9	4.3744295263	-0.3054475187	0.1025403660
O10	3.2653352411	1.6534984578	0.1068092307
O11	-2.7276618076	-1.9223793917	0.1071114534
O12	-1.6184673215	-3.8812573084	0.1025393895
C13	-3.9659891870	-2.6542670487	0.1071628757
C14	5.6128092390	0.4263452784	0.1025122770
H15	3.0024567736	-2.2945734468	0.1004593497
H16	0.8679757121	-3.5893456188	0.1004719167
H17	-1.3556885686	0.0668513463	0.1090157947
H18	0.7788075811	1.3616393204	0.1089881893
H19	-4.7493127699	-1.8998054487	0.1093306820
H20	-4.0378068553	-3.2822625103	-0.7821032799
H21	-4.0358903329	-3.2853807007	0.9943712043
H22	6.3960719380	-0.3281796450	0.1005194597
H23	5.6828462634	1.0573339064	-0.7847736017
H24	5.6845908584	1.0544499693	0.9917034586

#####mol\_reduced#####

24

structure

C1	2.0469406865	-1.7950445507	0.1023803098
C2	0.8771179905	-2.5093658385	0.1023621622
C3	-0.3975545068	-1.8632153619	0.1047515923
C4	-0.4001555712	-0.4327019651	0.1071993524
C5	0.7696695453	0.2816297423	0.1072276251
C6	2.0443432418	-0.3645271273	0.1048173089
C7	3.2355155499	0.4359357487	0.1049367933
C8	-1.5887088596	-2.6636993161	0.1045847985
O9	4.4073092435	-0.3313399994	0.1024101014
O10	3.3158910953	1.6647292836	0.1069333354
O11	-2.7605293060	-1.8964607689	0.1070677405
O12	-1.6690462918	-3.8924937590	0.1025755350
C13	-3.9595037604	-2.6511629768	0.1070379131
C14	5.6063203466	0.4233034476	0.1023555093
H15	2.9985669760	-2.3128623699	0.1005267529
H16	0.8919322815	-3.5936762864	0.1005069218
H17	-1.3517857518	0.0851052740	0.1090526376
H18	0.7548312066	1.3659368601	0.1090929476
H19	-4.7734956633	-1.9230450785	0.1090830066
H20	-4.0349494861	-3.2918704876	-0.7779399174
H21	-4.0331408974	-3.2948113851	0.9900325654
H22	6.4202747226	-0.3048565835	0.1002857758
H23	5.6799417831	1.0669218726	-0.7806621005
H24	5.6818450625	1.0640293412	0.9873126559

#####mol\_double\_reduced#####

24

structure

C1	2.0505022131	-1.7988066555	0.1023239959
C2	0.8935322559	-2.5122144580	0.1022506406
C3	-0.4292388579	-1.8909446452	0.1046482446

C4	-0.4036751292	-0.4289648695	0.1071483818
C5	0.7532571400	0.2844124494	0.1072184588
C6	2.0760744475	-0.3369202701	0.1048234660
C7	3.2230147040	0.4500510956	0.1050322686
C8	-1.5762122738	-2.6778177024	0.1044431204
O9	4.4578813547	-0.3472998046	0.1024405364
O10	3.3755117747	1.6984030367	0.1070209464
O11	-2.8111031862	-1.8804311250	0.1070129301
O12	-1.7287041076	-3.9261656132	0.1024707210
C13	-3.9775183883	-2.6491508019	0.1072479152
C14	5.6243125838	0.4214105901	0.1024816765
H15	3.0029808923	-2.3227923548	0.1004721998
H16	0.9243798498	-3.6000122607	0.1003426356
H17	-1.3562822794	0.0947588233	0.1090137225
H18	0.7224783832	1.3721913824	0.1091253833
H19	-4.8202882071	-1.9428094243	0.1091766462
H20	-4.0620678200	-3.3044618855	-0.7742916963
H21	-4.0601229704	-3.3069180528	0.9871509814
H22	6.4670558375	-0.2849492203	0.1004394504
H23	5.7069469988	1.0793846223	-0.7772566533
H24	5.7087945791	1.0764967891	0.9841975317

#####mol129#####

#####mol#####

30

structure

C1	2.0595919729	-1.7609214789	0.1128059215
C2	0.8876460411	-2.5044899370	0.1127771167
C3	-0.3545157646	-1.8623924487	0.1092565568
C4	-0.4150025169	-0.4645318892	0.1057381776
C5	0.7569443778	0.2790370944	0.1057137979
C6	1.9991110672	-0.3630557664	0.1092495024
C7	3.2242736477	0.4920770665	0.1090067575
C8	-1.5797122986	-2.7174670107	0.1094353237
O9	4.3592322082	-0.2352135700	0.1131891462
O10	3.2085206581	1.7007340099	0.1054688051
O11	-2.7146105008	-1.9900723905	0.1064850139
O12	-1.5640263343	-3.9261252359	0.1119383189
C13	-3.9533539921	-2.7409920297	0.1063202092
C14	5.5978418291	0.5159345758	0.1132912027
C15	-5.0919794515	-1.7426095881	0.1044712229
C16	6.7366630647	-0.4821971669	0.1197812791
H17	3.0223799148	-2.2534539606	0.1155366723
H18	0.9116675485	-3.5867898535	0.1154692544
H19	-1.3777877193	0.0280055920	0.1030363336
H20	0.7329241888	1.3613377371	0.1029850423
H21	-3.9696141334	-3.3863660385	-0.7749657019
H22	-3.9709280066	-3.3846391399	0.9888285395
H23	5.6167298931	1.1570927808	-0.7710142929
H24	5.6125331235	1.1638123821	0.9927519920

H25	-6.0478930320	-2.2728556660	0.1041773679
H26	-5.0536043829	-1.1047660783	0.9901973762
H27	-5.0521640050	-1.1063893601	-0.7823586942
H28	7.6924555949	0.0482658122	0.1199598361
H29	6.6956409059	-1.1158108906	1.0084192691
H30	6.6997701718	-1.1226483804	-0.7641230532

#####mol\_reduced#####

30

structure

C1	2.0575309505	-1.7722158708	0.1130115807
C2	0.9003235703	-2.5066923205	0.1130394487
C3	-0.3854277561	-1.8829347247	0.1095921003
C4	-0.4129767612	-0.4527929854	0.1060998168
C5	0.7442423520	0.2817008498	0.1060617726
C6	2.0299935827	-0.3420820647	0.1095078901
C7	3.2059070968	0.4803396014	0.1092870423
C8	-1.5612819347	-2.7054593217	0.1097801493
O9	4.3933816417	-0.2647582967	0.1129897269
O10	3.2617829868	1.7103034476	0.1063208953
O11	-2.7488929000	-1.9605693351	0.1062191650
O12	-1.6170010009	-3.9354249644	0.1126183154
C13	-3.9443788599	-2.7290716133	0.1060842618
C14	5.5890190537	0.5034899590	0.1129572428
C15	-5.1131034146	-1.7574523407	0.1031181568
C16	6.7574924136	-0.4684191793	0.1185400845
H17	3.0176314853	-2.2740527472	0.1156658487
H18	0.9339940250	-3.5905610897	0.1157056356
H19	-1.3730781086	0.0490340099	0.1034447087
H20	0.7105666551	1.3655658183	0.1033845736
H21	-3.9721655961	-3.3847999240	-0.7717137868
H22	-3.9741880505	-3.3819549415	0.9859098393
H23	5.6197876895	1.1548993813	-0.7679499307
H24	5.6161201446	1.1606583371	0.9896716733
H25	-6.0643845649	-2.3002279919	0.1028081893
H26	-5.0812300444	-1.1141134358	0.9863895277
H27	-5.0790813273	-1.1168906293	-0.7820896400
H28	7.7089049791	0.0741231219	0.1186862188
H29	6.7225781271	-1.1074353524	1.0048309584
H30	6.7261960865	-1.1132898344	-0.7636363150

#####mol\_double\_reduced#####

30

structure

C1	2.0611419561	-1.7763104200	0.1134525814
C2	0.9167335390	-2.5091960459	0.1134725078
C3	-0.4162538740	-1.9103155826	0.1099513748
C4	-0.4166238382	-0.4484493665	0.1062968785
C5	0.7277629650	0.2844035939	0.1062890695
C6	2.0608148324	-0.3145690583	0.1099049103
C7	3.1914807930	0.4939690615	0.1097930659

C8	-1.5468150107	-2.7189274713	0.1102969885
O9	4.4462409916	-0.2838640550	0.1141087021
O10	3.3237301412	1.7432356372	0.1068590557
O11	-2.8018427889	-1.9414410317	0.1068660272
O12	-1.6787251944	-3.9682285738	0.1131170903
C13	-3.9619152697	-2.7199856828	0.1024303742
C14	5.6066408321	0.4941633506	0.1095327279
C15	-5.1583161972	-1.7713282393	0.1039138912
C16	6.8025484614	-0.4550590503	0.1192922774
H17	3.0218360571	-2.2845015573	0.1161751213
H18	0.9662760581	-3.5961260538	0.1162132168
H19	-1.3774651002	0.0594373233	0.1035080766
H20	0.6783255587	1.3713181999	0.1035131013
H21	-4.0049548953	-3.3822929158	-0.7769838143
H22	-4.0072013439	-3.3884250387	0.9769010521
H23	5.6526745356	1.1521966175	-0.7729348790
H24	5.6494824037	1.1667610855	0.9809345205
H25	-6.1073184838	-2.3254859943	0.1004132023
H26	-5.1324688979	-1.1281342613	0.9893065184
H27	-5.1297697816	-1.1217111348	-0.7766934842
H28	7.751852912	0.0985741327	0.1161577591
H29	6.7735488992	-1.0940445801	1.0076297841
H30	6.7764096639	-1.1088321555	-0.7583084581

#####mol130#####

#####mol#####

30

structure

C1	5.5796141078	-1.0983584722	0.1361620007
C2	4.3787662324	-1.7909067470	0.1311894411
C3	4.3658592368	-3.1980371333	0.1106707908
C4	5.5923393622	-3.8900045706	0.0950206492
C5	6.7890663427	-3.1935570074	0.0996025474
C6	6.7937135987	-1.7943466328	0.1202863474
C7	3.1351661144	-3.9081813554	0.1064249797
C8	2.0860973910	-4.5129226720	0.1033306217
C9	0.8539693489	-5.2206708967	0.1012591598
C10	0.8367759947	-6.6277175657	0.1271281441
C11	-0.3662489927	-7.3166722484	0.1258087059
C12	-1.5780669684	-6.6171018580	0.0981384594
C13	-1.5690873306	-5.2180895326	0.0719769945
C14	-0.3703454808	-4.5252524509	0.0736506041
C15	-2.8939317793	-7.3078223568	0.0952602877
O16	-3.9661770812	-6.7521870645	0.0703724816
O17	-2.7807818942	-8.6585499331	0.1241770345
C18	8.1071423097	-1.0987872274	0.1245189767
O19	7.9882537574	0.2516139675	0.1471300544
O20	9.1819068852	-1.6499211636	0.1098454731
H21	5.5843545035	-0.0167551874	0.1522764809
H22	3.4386584007	-1.2538473207	0.1433409552

H23	5.5887317746	-4.9726246047	0.0789260815
H24	7.7374467924	-3.7157517434	0.0873149689
H25	1.7751177014	-7.1675644282	0.1484561302
H26	-0.3744425157	-8.3981845710	0.1461469069
H27	-2.5157913012	-4.6931721004	0.0505692527
H28	-0.3634686773	-3.4427038091	0.0534320693
H29	-3.6846200811	-9.0053199472	0.1197782056
H30	8.8907031230	0.6019994079	0.1479793989

#####mol\_reduced#####

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structure

C1	5.5819025060	-1.0931542949	0.1180929069
C2	4.3892298132	-1.7769385292	0.1125336608
C3	4.3477542917	-3.2055341483	0.1104375238
C4	5.6050238203	-3.8871963724	0.1136446667
C5	6.7921788537	-3.1966512679	0.1188115517
C6	6.8216416003	-1.7799109416	0.1215196379
C7	3.1406736430	-3.8997197638	0.1061036549
C8	2.0754604460	-4.5123768518	0.1028867365
C9	0.8684625798	-5.2067331859	0.1011236262
C10	0.8269354525	-6.6353563126	0.1087977460
C11	-0.3657990397	-7.3191239171	0.1082098091
C12	-1.6054985036	-6.6323086514	0.0994571043
C13	-1.5759242434	-5.2156338382	0.0913345643
C14	-0.3887649140	-4.5251275290	0.0922326019
C15	-2.8852636586	-7.3108179929	0.0983851271
O16	-3.9936958618	-6.7923164055	0.0902328411
O17	-2.7855018130	-8.6890708985	0.1078705845
C18	8.1011583843	-1.1009132936	0.1277460167
O19	8.0004993320	0.2772977975	0.1311085678
O20	9.2099810891	-1.6186613564	0.1302263149
H21	5.5829995516	-0.0100542514	0.1200293459
H22	3.4508587332	-1.2337875207	0.1100159443
H23	5.6045266786	-4.9714283589	0.1118478734
H24	7.7383065739	-3.7254834723	0.1210206156
H25	1.7652935174	-7.1784874183	0.1154876678
H26	-0.3669896386	-8.4022119964	0.1145496832
H27	-2.5220285441	-4.6868026482	0.0843308091
H28	-0.3882867721	-3.4409140925	0.0860239195
H29	-3.7049765838	-8.9854351473	0.1059223564
H30	8.9197895948	0.5742060626	0.1350747020

#####mol\_double\_reduced#####

30

structure

C1	5.5908060943	-1.0843454848	0.1130755293
C2	4.4052054479	-1.7616994849	0.1087946996
C3	4.3360647330	-3.2125724938	0.1130201240
C4	5.6260938291	-3.8818998278	0.1217254469
C5	6.8045246693	-3.1944651709	0.1259394063



C6	6.8591052142	-1.7590570144	0.1220337458
C7	3.1491994908	-3.8948881904	0.1092378771
C8	2.0668579269	-4.5175708618	0.1059558705
C9	0.8801007837	-5.2001002359	0.1039203735
C10	0.8110712736	-6.6510427216	0.1051854627
C11	-0.3745065320	-7.3285207293	0.1031773714
C12	-1.6429000212	-6.6539075732	0.0996368481
C13	-1.5883725588	-5.2184929762	0.0982375239
C14	-0.4100036434	-4.5309651615	0.1001925200
C15	-2.8926215506	-7.3186800877	0.0974320372
O16	-4.0390089427	-6.8369374911	0.0943574519
O17	-2.8088055443	-8.7294213599	0.0990002831
C18	8.1086320020	-1.0939458879	0.1268719245
O19	8.0241709797	0.3167570624	0.1222183267
O20	9.2552687083	-1.5750493888	0.1345178442
H21	5.5862577065	0.0010120810	0.1096388771
H22	3.4678215602	-1.2123585618	0.1019909453
H23	5.6309967326	-4.9684051565	0.1248688533
H24	7.7494399471	-3.7297802061	0.1324800373
H25	1.7485593191	-7.2002273105	0.1077838534
H26	-0.3698191950	-8.4139025225	0.1042745017
H27	-2.5333206805	-4.6831998283	0.0955148097
H28	-0.4151179842	-3.4444552749	0.0989354542
H29	-3.7435866968	-8.9691383068	0.0969988945
H30	8.9588297945	0.5568649164	0.1264096807

#####mol131#####

#####mol#####

24

structure

C1	-1.2225070178	-0.2257772305	0.1035345133
C2	-1.2179440773	-1.6393972693	0.1102872757
C3	-2.5064112783	-2.3740082713	0.1078315603
O4	-3.6627026195	-1.6056452042	0.0987700512
C5	-3.7251246972	-0.2186238573	0.0917976754
C6	-2.4315061354	0.5067632100	0.0944019275
C7	-2.4111980214	1.8892964075	0.0879170142
C8	-1.1875211594	2.5812444852	0.0903246289
C9	0.0076326808	1.8860002153	0.0991989874
C10	0.0120971662	0.4723713097	0.1059685175
C11	1.2210676892	-0.2601968051	0.1151082723
C12	1.2008263853	-1.6427302583	0.1215581069
C13	-0.0228173190	-2.3346636610	0.1191338913
C14	1.2961271004	2.6205606647	0.1016784339
O15	2.4524171135	1.8521423892	0.1107784196
C16	2.5146977333	0.4651736644	0.1177553607
O17	-4.8003409381	0.3017673947	0.0842135011
O18	-2.6146497392	-3.5636495819	0.1130526651
O19	3.5898590847	-0.0553447111	0.1253684460
O20	1.4044450454	3.8101948538	0.0964529172

H21	-3.3508023825	2.4271957509	0.0809760721
H22	-1.1642716541	3.6636846220	0.0852810352
H23	2.1404837068	-2.1805348427	0.1284848243
H24	-0.0463193759	-3.4170971258	0.1241516141

#####mol\_reduced#####

24

structure

C1	-1.2290665222	-0.2294880923	0.1035380910
C2	-1.2216699275	-1.6442752452	0.1103131994
C3	-2.4830529693	-2.3680185678	0.1079148530
O4	-3.6441896869	-1.5951236182	0.0987991130
C5	-3.7079434639	-0.2016112393	0.0917731801
C6	-2.4375825304	0.5061641400	0.0943819252
C7	-2.4111881801	1.9162519412	0.0878051519
C8	-1.2105396287	2.5951231030	0.0901728025
C9	0.0113205463	1.8908428715	0.0992196487
C10	0.0186927671	0.4760328420	0.1060006639
C11	1.2271996152	-0.2596153394	0.1151437837
C12	1.2008450872	-1.6696978506	0.1217074802
C13	0.0001846482	-2.3485733220	0.1193443772
C14	1.2726588627	2.6145721060	0.1016066416
O15	2.4338514268	1.8416255104	0.1107134628
C16	2.4976062971	0.4482018730	0.1177323702
O17	-4.8088917509	0.3009623101	0.0841287549
O18	-2.6197053413	-3.5705464619	0.1130537318
O19	3.5985331207	-0.0544537749	0.1253546930
O20	1.4093840703	3.8170852676	0.0964610141
H21	-3.3566390249	2.4438619942	0.0808928299
H22	-1.1752136205	3.6772630230	0.0851896870
H23	2.1463183208	-2.1972649838	0.1286002548
H24	-0.0351859991	-3.4307152642	0.1243169502

#####mol\_double\_reduced#####

24

structure

C1	-1.2355081085	-0.2331779867	0.1035000019
C2	-1.2270051414	-1.6516811654	0.1102944656
C3	-2.4663795249	-2.3668685813	0.1079363174
O4	-3.6311683483	-1.5878930436	0.0988093994
C5	-3.6983756781	-0.1876148872	0.0918082666
C6	-2.4467957412	0.5053920898	0.0943268658
C7	-2.4148623734	1.9423493519	0.0876325093
C8	-1.2310593486	2.6117403060	0.0899600256
C9	0.0167312926	1.8983241764	0.0991793759
C10	0.0251581126	0.4797149615	0.1059966563
C11	1.2363083712	-0.2588174234	0.1151921769
C12	1.2045198295	-1.6957457364	0.1218702152
C13	0.0206585660	-2.3651491017	0.1195073840
C14	1.2558464229	2.6135041046	0.1015236316
O15	2.4208875437	1.8341977309	0.1107290586

C16	2.4880366065	0.4343673629	0.1177806170
O17	-4.8266703475	0.2986057970	0.0842391952
O18	-2.6307946542	-3.5844725042	0.1129833457
O19	3.6161822315	-0.0522459842	0.1254404652
O20	1.4206923854	3.8310254730	0.0964218504
H21	-3.3665237193	2.4622618553	0.0807226594
H22	-1.1860505248	3.6952241486	0.0850069106
H23	2.1562507301	-2.2155306405	0.1287921894
H24	-0.0244513878	-3.4486443621	0.1244261381

#####mol132#####

#####mol#####

28

structure

C1	0.1908973472	-0.2486329322	0.2432933525
C2	0.2331472203	-1.6671582485	0.2740933922
C3	-1.0905649214	-2.3830190892	0.4196361703
O4	-2.1369548588	-1.6281540673	-0.1858636730
C5	-2.3253985657	-0.3457391535	0.4063785896
C6	-1.0388868807	0.4609556764	0.2987412147
C7	-1.0422424522	1.8400786073	0.2672320990
C8	0.1651489310	2.5581642589	0.1804979673
C9	1.3737140660	1.8917475617	0.1206839055
C10	1.4083082205	0.4782025659	0.1477746194
C11	2.6334405136	-0.2249006766	0.0796974477
C12	2.6426931021	-1.6064800007	0.0997571912
C13	1.4390530517	-2.3294356566	0.1968885809
C14	2.6370262076	2.6541324426	0.0268629630
O15	3.8101357612	1.9120617759	-0.0344038704
C16	3.9037892703	0.5242608831	-0.0156375075
O17	4.9934943494	0.0341899692	-0.0763385534
O18	2.7230621157	3.8473194164	0.0002857271
O19	-1.0217375284	-3.6242033451	-0.1960007823
O20	-3.4178609824	0.2623204513	-0.1966768451
H21	-1.3288546286	-2.4844912536	1.4956618572
H22	-2.6028680141	-0.4659296447	1.4642303204
H23	-1.9858299381	2.3702224652	0.3053312945
H24	0.1655709911	3.6407935323	0.1565594118
H25	3.5934098702	-2.1211491643	0.0373640142
H26	1.4528927281	-3.4112997930	0.1990776777
H27	-1.8634426126	-4.0714194227	-0.0546448643
H28	-3.2184940124	0.3543353170	-1.1370798403

#####mol\_reduced#####

28

structure

C1	0.1906100851	-0.2544989355	0.2374366385
C2	0.2463268930	-1.6690782813	0.2725000346
C3	-1.0641470439	-2.3788395488	0.4602094866
O4	-2.1424914793	-1.6607003408	-0.1388180524
C5	-2.3239528579	-0.3424316840	0.3890387559

C6	-1.0409042094	0.4505961784	0.3029107571
C7	-1.0488508634	1.8554953313	0.3004141929
C8	0.1296554739	2.5750854400	0.2154615791
C9	1.3721527763	1.9043349656	0.1292485958
C10	1.4165497736	0.4868680369	0.1396514939
C11	2.6439510898	-0.2158791666	0.0617646694
C12	2.6571440176	-1.6288115631	0.0817432907
C13	1.4730110699	-2.3384118427	0.1903367852
C14	2.6024313197	2.6583887476	0.0342000755
O15	3.7831003416	1.9148205022	-0.0443342197
C16	3.8861211494	0.5237019489	-0.0360733107
O17	5.0044833642	0.0529637302	-0.1100619487
O18	2.7126024321	3.8696514480	0.0158736601
O19	-1.0331189760	-3.6513406898	-0.1287340282
O20	-3.3870170812	0.2456259546	-0.3133199536
H21	-1.2959759650	-2.4752320594	1.5418252742
H22	-2.6915821480	-0.4264678543	1.4249788246
H23	-2.0000279279	2.3744861831	0.3586305214
H24	0.1321427555	3.6578444808	0.2088071863
H25	3.6133683554	-2.1314778054	0.0101033596
H26	1.4806771906	-3.4220255563	0.2007033366
H27	-1.9144954011	-4.0211010585	-0.0090540013
H28	-3.0308182018	0.4811975170	-1.1793267537

#####mol\_double\_reduced#####

28

structure

C1	0.1835811064	-0.2631492702	0.2143039276
C2	0.2557374453	-1.6756814660	0.2401939714
C3	-1.0284210293	-2.3513384391	0.5611847540
O4	-2.1576655788	-1.7074062332	-0.0442645228
C5	-2.3418181641	-0.3256749888	0.3019109116
C6	-1.0536305275	0.4354416588	0.3080281201
C7	-1.0589438826	1.8642517139	0.4028453600
C8	0.0962424887	2.5897290677	0.3430765191
C9	1.3668509727	1.9182179022	0.1777947640
C10	1.4165138797	0.4950769721	0.1220720177
C11	2.6475681548	-0.2044194751	-0.0017891905
C12	2.6703395172	-1.6462910862	-0.0061654331
C13	1.5015636117	-2.3477163213	0.1305834777
C14	2.5714014929	2.6702652396	0.0893068752
O15	3.7568013553	1.9270544358	-0.0566026140
C16	3.8680330968	0.5352455268	-0.1001399308
O17	5.0121982180	0.0841316538	-0.2166054709
O18	2.7076119814	3.8990253061	0.1220669598
O19	-1.0696801431	-3.6960609408	0.1062856854
O20	-3.2832327442	0.1934247201	-0.6428830420
H21	-1.2248858499	-2.3539861805	1.6631512138
H22	-2.9111838236	-0.2798750545	1.2522968673
H23	-2.0175710639	2.3719971850	0.5039958546

H24	0.1028445235	3.6719106839	0.4064802209
H25	3.6309610198	-2.1364574415	-0.1135306057
H26	1.5067988015	-3.4350038017	0.1412901400
H27	-1.9910586675	-3.9525054269	0.2275807345
H28	-2.7177611366	0.4726455272	-1.3764419117

#####mol133#####

#####mol#####

32

structure

C1	0.2443839973	-0.2279398942	-0.1118394641
C2	-0.9846815532	0.4836958996	-0.0793705859
C3	-2.2487595401	-0.3404462072	-0.1425242188
O4	-2.0570230253	-1.6103908104	0.4764597417
C5	-1.0490130227	-2.3975041803	-0.1548225244
C6	0.2752099513	-1.6497706776	-0.1395772407
C7	1.4832834856	-2.3081430972	-0.1536115716
C8	2.6998514269	-1.5898778418	-0.1473744304
C9	2.6989726732	-0.2157999829	-0.1262030945
C10	1.4691412744	0.4971260136	-0.1007052495
C11	1.4345751563	1.9174248155	-0.0461321484
C12	0.2294437064	2.5760201576	0.0073398458
C13	-0.9863029783	1.8561641056	-0.0119313814
C14	3.9692061344	0.6027885345	-0.1451473296
O15	3.7777900660	1.8402787497	0.5372544612
C16	2.7615798951	2.6403560824	-0.0656676545
O17	-3.2801360726	0.3193192214	0.5166181090
O18	-0.9993091703	-3.6341037056	0.4811112162
O19	2.6609341549	3.8356547242	0.6374845655
O20	4.9939029137	-0.0979600139	0.4819481345
H21	-2.5144998752	-0.5236537775	-1.2016438150
H22	-1.3539016695	-2.6159447174	-1.1891890204
H23	1.4976138844	-3.3916412629	-0.1606785388
H24	3.6429478821	-2.1214145340	-0.1412162697
H25	0.2173659011	3.6560695035	0.0809178601
H26	-1.9295820874	2.3844686581	0.0434810442
H27	4.2395753946	0.8360147819	-1.1936443635
H28	3.0624792809	2.8279780507	-1.1149980826
H29	-4.0690598081	-0.2281583969	0.4382369664
H30	-0.7295470315	-3.4740713898	1.3943931565
H31	3.5111074763	4.2839741135	0.5741855599
H32	5.7923656562	0.4374400090	0.4219749137

#####mol\_reduced#####

32

structure

C1	0.2314199288	-0.2294429081	-0.0760225931
C2	-0.9856819653	0.4963822251	-0.0677334514
C3	-2.2336698804	-0.3212956852	-0.2031983481
O4	-2.1042442251	-1.6018675648	0.4141430132
C5	-1.0423192183	-2.4060831172	-0.1144244502

C6	0.2606213808	-1.6507593004	-0.1254277824
C7	1.4955127588	-2.3331674070	-0.2122804205
C8	2.6906975907	-1.6331723819	-0.2133424969
C9	2.6961143143	-0.2283713636	-0.1211079480
C10	1.4742545033	0.4973906553	-0.0582161401
C11	1.4359385161	1.9140237360	-0.0052230418
C12	0.2082978608	2.6013868141	0.0150045017
C13	-0.9883322882	1.9005047556	-0.0200827730
C14	3.9607030314	0.5715653625	-0.1718429547
O15	3.8149811104	1.8378394752	0.4789510613
C16	2.7511537085	2.6336368032	-0.0500870617
O17	-3.3321045151	0.3143925397	0.4070601108
O18	-0.9910048899	-3.5806467221	0.6640920922
O19	2.7060655546	3.8174031431	0.7124105175
O20	5.0142050601	-0.1048136695	0.4748603201
H21	-2.4700434466	-0.5003853396	-1.2759598257
H22	-1.3424546765	-2.7634969255	-1.1155861076
H23	1.4979665026	-3.4175803905	-0.2601328238
H24	3.6363744578	-2.1621870221	-0.2570561299
H25	0.2104139386	3.6836597750	0.0801672678
H26	-1.9360716359	2.4260221743	0.0101441088
H27	4.2658110298	0.7798174100	-1.2223130945
H28	3.0276172011	2.8946445857	-1.0959011792
H29	-4.0594805923	-0.3142168494	0.3420917190
H30	-0.5149723877	-3.3268685935	1.4653674823
H31	3.5826255584	4.2107609541	0.6386816642
H32	5.7850033576	0.4675734338	0.3911474584

#####mol\_double\_reduced#####

32

structure

C1	0.2086915125	-0.2161063521	0.0211013046
C2	-1.0085298221	0.5127319651	0.0454720969
C3	-2.2428902342	-0.2797894427	-0.0961428987
O4	-2.1467577953	-1.6048017261	0.4516866074
C5	-1.0124571277	-2.4132935071	0.1335216117
C6	0.2577872189	-1.6375698106	0.0394239419
C7	1.5091685166	-2.3262079242	-0.1260676185
C8	2.6792298314	-1.6285372865	-0.2632431772
C9	2.6743902027	-0.1902355722	-0.2457123350
C10	1.4611095145	0.5130543757	-0.0892751567
C11	1.4237756670	1.9411405074	-0.0721377149
C12	0.1654430407	2.6384061429	-0.1696783720
C13	-1.0121084047	1.9466516927	-0.1230930796
C14	3.9327615252	0.5619845600	-0.5410395234
O15	3.7072019885	1.9213952790	-0.9161598513
C16	2.7295717583	2.6093716415	-0.1460320888
O17	-3.3473058016	0.3303639836	0.5750381933
O18	-0.9623724282	-3.4321684413	1.1526942914
O19	3.3254854712	2.8024487604	1.2281687458

O20	4.9409992897	0.5274784553	0.5095101889
H21	-2.5720170111	-0.4054199280	-1.1709385241
H22	-1.2459639342	-3.0148893927	-0.7702391225
H23	1.5110830597	-3.4148149751	-0.1024814932
H24	3.6303301950	-2.1523438657	-0.3516483504
H25	0.1694643848	3.7263508619	-0.2586483758
H26	-1.9679487603	2.4618921582	-0.1673278597
H27	4.4669275624	0.1289473335	-1.3983630684
H28	2.6883744266	3.6131025937	-0.5840961091
H29	-4.1223234717	-0.1582654727	0.2599133385
H30	-0.4583513762	-2.9963839945	1.8546088001
H31	2.5934036385	2.4838967367	1.7738632164
H32	4.5593601158	1.1172193188	1.1761682078

#####mol134#####

#####mol#####

28

structure

C1	0.2042226393	-0.2262609044	0.1022839992
C2	-1.0093962230	0.5041780240	0.1044256237
C3	-2.2895843655	-0.2256676243	0.0988753550
O4	-2.2350439976	-1.6131829477	0.0917281311
C5	-1.0705845927	-2.3695567406	0.0893632188
C6	0.2112644803	-1.6426973741	0.0949127534
C7	1.4128925801	-2.3291442656	0.0929855652
C8	2.6315658624	-1.6362478722	0.0982581191
C9	2.6562288179	-0.2525982413	0.1054878098
C10	1.4425731176	0.4778011484	0.1076451319
C11	1.4354671611	1.8942317835	0.1150306748
C12	0.2338594442	2.5807205375	0.1169665174
C13	-0.9848071416	1.8878360433	0.1116702575
C14	3.9363962070	0.4772945751	0.1110027243
O15	3.8817770826	1.8647809907	0.1181674810
C16	2.7172737790	2.6211511706	0.1205762762
N17	-1.1394283627	-3.6307299353	0.0826711376
N18	-3.4086219172	0.3600346500	0.1003939460
N19	2.7860632814	3.8823278253	0.1272972544
N20	5.0554606726	-0.1083695578	0.1094422862
H21	-4.1743084997	-0.3135996651	0.0958370262
H22	3.7565002746	4.1958929571	0.1302623967
H23	5.8211006045	0.5653175859	0.1139779548
H24	-2.1098910560	-3.9442311736	0.0796990911
H25	1.3925982863	-3.4110375417	0.0873219811
H26	3.5715656500	-2.1722946755	0.0967493780
H27	0.2542369748	3.6626195826	0.1226480582
H28	-1.9249062316	2.4236991579	0.1131692708

#####mol\_reduced#####

28

structure

C1	0.1982295230	-0.2296407348	0.1022578857
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C2	-1.0138407148	0.5052712380	0.1044389555
C3	-2.2750460417	-0.2101160937	0.0989959950
O4	-2.2170055411	-1.6028893049	0.0918219843
C5	-1.0497240477	-2.3649709378	0.0894144088
C6	0.2099588327	-1.6470323436	0.0948832332
C7	1.4360648339	-2.3455494726	0.0928966898
C8	2.6338770744	-1.6645404003	0.0980806917
C9	2.6606376279	-0.2536810104	0.1054794736
C10	1.4485431006	0.4812207099	0.1076587034
C11	1.4367804868	1.8985916825	0.1150274475
C12	0.2106881192	2.5971380592	0.1170066271
C13	-0.9871140200	1.9161229895	0.1118317784
C14	3.9218084487	0.4617046715	0.1109323789
O15	3.8637213288	1.8544954858	0.1180933410
C16	2.6964677212	2.6165543942	0.1204945377
N17	-1.1576990366	-3.6405146511	0.0825841716
N18	-3.4264401881	0.3493226741	0.1003409511
N19	2.8044203559	3.8920969174	0.1273202191
N20	5.0732365549	-0.0976804454	0.1096101282
H21	-4.1474333507	-0.3723263507	0.0955904077
H22	3.7932711587	4.1426830510	0.1299766041
H23	5.7941997859	0.6239989014	0.1143599650
H24	-2.1465477318	-3.8910999540	0.0799190989
H25	1.4041306341	-3.4275533557	0.0871964476
H26	3.5800072578	-2.1904767290	0.0966227535
H27	0.2426781032	3.6791381394	0.1226998396
H28	-1.9332607915	2.4420212559	0.1132954071

#####mol\_double\_reduced#####

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structure

C1	0.1924594770	-0.2329912082	0.1022106833
C2	-1.0216274837	0.5056806433	0.1043892103
C3	-2.2668861341	-0.1971216731	0.0990267802
O4	-2.2033575759	-1.5951180661	0.0918611628
C5	-1.0342919468	-2.3647729035	0.0894572644
C6	0.2062988965	-1.6541018643	0.0948357394
C7	1.4558484075	-2.3631963235	0.0928467357
C8	2.6389276308	-1.6905148895	0.0979437859
C9	2.6685473942	-0.2540953180	0.1054663978
C10	1.4543511792	0.4844927706	0.1076766717
C11	1.4403902778	1.9055311760	0.1151014594
C12	0.1909389062	2.6147542575	0.1170830818
C13	-0.9921487836	1.9420673049	0.1119355365
C14	3.9136703037	0.4486860810	0.1108195911
O15	3.8500185885	1.8468110843	0.1180645331
C16	2.6810675658	2.6162983516	0.1205387155
N17	-1.1797533620	-3.6570018074	0.0825552851
N18	-3.4516680462	0.3389097436	0.1001822194
N19	2.8262557377	3.9085683164	0.1275563132



N20	5.0985768228	-0.0870610110	0.1095993524
H21	-4.1288260109	-0.4256442759	0.0953046635
H22	3.8295790997	4.0994824378	0.1298918578
H23	5.7755201726	0.6776752698	0.1145136850
H24	-2.1831061344	-3.8477192328	0.0802241092
H25	1.4154675857	-3.4464968670	0.0871631562
H26	3.5904574675	-2.2099229545	0.0965360162
H27	0.2315791159	3.6980363114	0.1228022028
H28	-1.9438336419	2.4611887602	0.1133360090

#####mol135#####

#####mol#####

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structure

C1	0.2003022833	-0.2250577975	0.1041843193
C2	-1.0127957942	0.5095104131	0.1020287570
C3	-2.3148586118	-0.2109254414	0.0992401610
N4	-2.2187808198	-1.6019949551	0.0989954365
C5	-1.0717171672	-2.3948888069	0.1010022740
C6	0.2124612728	-1.6431551217	0.1037664076
C7	1.4092562076	-2.3327600221	0.1059168022
C8	2.6301981393	-1.6378697175	0.1085369301
C9	2.6484199046	-0.2567065346	0.1089936522
C10	1.4352690734	0.4778035683	0.1068327131
C11	1.4230697392	1.8959088429	0.1072444643
C12	0.2262980166	2.5855614471	0.1051142076
C13	-0.9946098376	1.8906754403	0.1025016251
C14	3.9504492988	0.4637607689	0.1117759204
N15	3.8543112055	1.8548538163	0.1119876468
C16	2.7072395074	2.6476701550	0.1099876536
O17	-1.1475725243	-3.6048062173	0.1004689842
O18	-3.3939957857	0.3414614810	0.0972871508
O19	2.7830024027	3.8576147382	0.1105096256
O20	5.0296125051	-0.0885725218	0.1137533489
H21	-3.0996390919	-2.1033939272	0.0970991467
H22	1.3843754871	-3.4152777495	0.1055350106
H23	3.5735138626	-2.1694952043	0.1102310008
H24	0.2512781191	3.6680793373	0.1055040882
H25	-1.9380483727	2.4220858958	0.1008196570
H26	4.7351426975	2.3562929167	0.1138565203

#####mol\_reduced#####

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structure

C1	0.1938351968	-0.2287137188	0.1041776056
C2	-1.0196038816	0.5101687420	0.1020100243
C3	-2.2976876500	-0.1943930095	0.0992599805
N4	-2.1941537120	-1.5879476436	0.0990536598
C5	-1.0486722427	-2.3884956079	0.1010778842
C6	0.2095626086	-1.6493216926	0.1037754048
C7	1.4322775350	-2.3473572733	0.1059557813

C8	2.6309874558	-1.6651362370	0.1085188261
C9	2.6552087755	-0.2573630097	0.1090099441
C10	1.4417252595	0.4814951927	0.1068529140
C11	1.4259720204	1.9020806843	0.1072555712
C12	0.2032749820	2.6001576798	0.1050765877
C13	-0.9954318967	1.9179178049	0.1025087676
C14	3.9332427281	0.4471858629	0.1117263441
N15	3.8296871944	1.8407941935	0.1119476414
C16	2.6842415561	2.6412961544	0.1099474443
O17	-1.1594404118	-3.6132848471	0.1004984361
O18	-3.4074062502	0.3356153755	0.0972039471
O19	2.7949083577	3.8660949171	0.1105387449
O20	5.0430154511	-0.0827147826	0.1137413402
H21	-3.0734339586	-2.0884586326	0.0971557876
H22	1.3958723484	-3.4298546378	0.1055385251
H23	3.5801973841	-2.1867587222	0.1102103020
H24	0.2397534568	3.6826474028	0.1054919960
H25	-1.9446875770	2.4394668318	0.1008153283
H26	4.7089835943	2.3412778006	0.1138381091

#####mol\_double\_reduced#####

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structure

C1	0.1874037560	-0.2324994075	0.1041550900
C2	-1.0296258250	0.5103516303	0.1019866047
C3	-2.2885872058	-0.1815084604	0.0992798849
N4	-2.1761371312	-1.5774434902	0.0990891713
C5	-1.0329638493	-2.3873264795	0.1010941590
C6	0.2044936333	-1.6584117060	0.1037515729
C7	1.4526949680	-2.3644315917	0.1060017929
C8	2.6351662895	-1.6913251544	0.1085377121
C9	2.6654640847	-0.2575301708	0.1090343362
C10	1.4482194994	0.4851092083	0.1068597279
C11	1.4309764999	1.9109363523	0.1072662963
C12	0.1829617820	2.6171414377	0.1050675481
C13	-0.9995355769	1.9440016103	0.1025281991
C14	3.9242334389	0.4343004025	0.1117129304
N15	3.8115901602	1.8304667751	0.1118993362
C16	2.6685204868	2.6399868352	0.1099015907
O17	-1.1792552664	-3.6291415868	0.1004328362
O18	-3.4306241176	0.3276733614	0.0971662621
O19	2.8141155118	3.8819158861	0.1105567169
O20	5.0665333466	-0.0743368384	0.1138101621
H21	-3.0544499652	-2.0778727077	0.0972070731
H22	1.4083052430	-3.4483658992	0.1055881824
H23	3.5897513627	-2.2067052024	0.1102685896
H24	0.2276484970	3.7010647022	0.1055220497
H25	-1.9542790779	2.4591145527	0.1008314716
H26	4.6898812122	2.3309352089	0.1137820476

#####mol136#####

#####mol#####

20

structure

C1	0.8280392856	-2.5484887646	0.0888247288
C2	-0.3429569301	-1.8014373439	0.0797740368
C3	-0.3416557798	-0.4034841527	0.0900904432
C4	0.8307547776	0.3411247623	0.1101345970
C5	2.0017589668	-0.4059227916	0.1191907744
C6	2.0004484447	-1.8038697426	0.1088791184
C7	-1.7634812239	0.0713105969	0.0759467772
N8	-2.5294191621	-1.1002429107	0.0577782449
C9	-1.7656606596	-2.2733486909	0.0586123878
C10	3.4222667069	-2.2786848443	0.1230476397
N11	4.1882199464	-1.1071454727	0.1412032938
C12	3.4244692892	0.0659704061	0.1403587096
O13	3.8461056733	1.1933698935	0.1539152149
O14	3.8417794995	-3.4069568443	0.1199276824
O15	-2.1830171568	1.1995761433	0.0790829219
O16	-2.1872816315	-3.4007548056	0.0450568577
H17	0.8270419569	-3.6314300828	0.0808363041
H18	0.8318036099	1.4240683391	0.1181124219
H19	-3.5391826550	-1.0991860866	0.0452343995
H20	5.1979839611	-1.1082111566	0.1537462934

#####mol\_reduced#####

20

structure

C1	0.8280319160	-2.5481531649	0.0888157764
C2	-0.3561987035	-1.8214922242	0.0794559247
C3	-0.3548773748	-0.3833962620	0.0901078354
C4	0.8307266789	0.3408027573	0.1101616641
C5	2.0150045472	-0.3858591133	0.1194950556
C6	2.0136655168	-1.8239398976	0.1089046872
C7	-1.7407871107	0.0831904165	0.0763598860
N8	-2.5054157403	-1.1002489653	0.0580683989
C9	-1.7429813221	-2.2852352343	0.0587636836
C10	3.3995636238	-2.2905687865	0.1227335047
N11	4.1642163552	-1.1071472991	0.1408757310
C12	3.4017930473	0.0778664102	0.1400993809
O13	3.8758402258	1.2072804978	0.1542613065
O14	3.8713846649	-3.4210012795	0.1203405784
O15	-2.2126518957	1.2135974271	0.0788969217
O16	-2.2169734346	-3.4146679233	0.0444909042
H17	0.8271774484	-3.6326529094	0.0808001935
H18	0.8319619356	1.4253074102	0.1181724396
H19	-3.5129903921	-1.0993534767	0.0455247245
H20	5.1717919083	-1.1080845535	0.1533855306

#####mol\_double\_reduced#####

20

structure

C1	0.8281094690	-2.5486119682	0.0888188985
C2	-0.3703169308	-1.8422985394	0.0791105626
C3	-0.3688802652	-0.3628084475	0.0900871546
C4	0.8306490481	0.3412083125	0.1101412287
C5	2.0291169722	-0.3651529339	0.1198162335
C6	2.0276983672	-1.8445469919	0.1089462180
C7	-1.7291759489	0.0969518584	0.0766600982
N8	-2.4895128055	-1.1001203985	0.0582848187
C9	-1.7314562684	-2.2988948088	0.0587491398
C10	3.3879879540	-2.3043061306	0.1225306525
N11	4.1483574684	-1.1072453850	0.1407076937
C12	3.3902091001	0.0915471473	0.1400236966
O13	3.9184109209	1.2234140431	0.1548091127
O14	3.9135138566	-3.4374738092	0.1207985728
O15	-2.2547197301	1.2300710208	0.0785976414
O16	-2.2596775391	-3.4307332390	0.0437479705
H17	0.8276819396	-3.6367119179	0.0807791846
H18	0.8319335757	1.4293065822	0.1181686217
H19	-3.4969761026	-1.0997440358	0.0457646724
H20	5.1558249101	-1.1076404411	0.1532369995

#####mol137#####

#####mol#####

30

structure

C1	-3.5872276938	-1.8905956751	0.0949798340
C2	-2.3657426733	-1.2216028021	0.1001853519
C3	-2.3165618565	0.1896496712	0.1052163194
C4	-3.4854463909	0.9468232648	0.1051326710
C5	-4.6975135149	0.2596273531	0.0998969456
C6	-4.7587654808	-1.1419102129	0.0948494055
N7	-0.9961172401	0.6147253280	0.1097776123
C8	-0.1507925535	-0.4749185218	0.1079487182
C9	-0.9825417575	-1.7150994398	0.1017122293
O10	-0.5406708811	-2.8586287430	0.0988011141
C11	1.2065179022	-0.4318939455	0.1112693851
N12	2.0519207075	-1.5214678632	0.1094982067
C13	3.3723528804	-1.0963138714	0.1141959506
C14	3.4214281844	0.3149480657	0.1192420059
C15	2.0381917588	0.8083222617	0.1175317872
O16	1.5962461765	1.9518238938	0.1203429574
C17	4.5413194560	-1.8533746746	0.1144098896
C18	5.7533264319	-1.1660683615	0.1197955197
C19	5.8144630675	0.2354710464	0.1248705415
C20	4.6428557283	0.9840512980	0.1246098392
H21	-3.6070573038	-2.9743500374	0.0911364423
H22	-3.4563513775	2.0299882742	0.1089892747
H23	-5.6206981002	0.8285489438	0.0997271092
H24	-5.7224110742	-1.6361940151	0.0908569490
H25	-0.6490495174	1.5636734688	0.1138972091

H26	1.7048775538	-2.4704210902	0.1053531608
H27	4.5123441913	-2.9365379478	0.1105354560
H28	6.6765676040	-1.7349064549	0.1200643206
H29	6.7780737428	0.7298280863	0.1289860059
H30	4.6625899122	2.0678045603	0.1284716888

#####mol\_reduced#####

30

structure

C1	-3.5742874862	-1.8832360144	0.0949652144
C2	-2.3448957747	-1.2237933048	0.1001749599
C3	-2.3094596949	0.2014665649	0.1052918649
C4	-3.4874386550	0.9504054865	0.1051830987
C5	-4.7022073364	0.2656349416	0.0999278879
C6	-4.7512292880	-1.1391869236	0.0948484162
N7	-0.9996230889	0.6082596212	0.1097823736
C8	-0.1622690409	-0.5060358343	0.1078336930
C9	-0.9615583790	-1.7128983693	0.1016666714
O10	-0.5337218803	-2.8970302296	0.0984413902
C11	1.2179564562	-0.4003065478	0.1114751485
N12	2.0551582379	-1.5147178349	0.1096429267
C13	3.3650497917	-1.1081098505	0.1142156531
C14	3.4006803706	0.3171464732	0.1192003869
C15	2.0174138510	0.8064565152	0.1175493971
O16	1.5897625109	1.9906460897	0.1205898258
C17	4.5429279043	-1.8572019779	0.1145002309
C18	5.7577872199	-1.1726072145	0.1197996204
C19	5.8070028846	0.2322108899	0.1247433711
C20	4.6301594757	0.9764164199	0.1244454586
H21	-3.5926406525	-2.9684952504	0.0910758281
H22	-3.4580301404	2.0354896541	0.1090747802
H23	-5.6284866558	0.8320863472	0.0997697511
H24	-5.7133862200	-1.6413209927	0.0908292305
H25	-0.6094977579	1.5421452289	0.1139714040
H26	1.6647822433	-2.4485227826	0.1054950206
H27	4.5133647478	-2.9422814207	0.1107004347
H28	6.6839888021	-1.7391890665	0.1200994408
H29	6.7692370063	0.7342009739	0.1287997888
H30	4.6486498945	2.0616738303	0.1282175838

#####mol\_double\_reduced#####

30

structure

C1	-3.5700449675	-1.8808267288	0.0950435534
C2	-2.3250975601	-1.2324506546	0.1002762394
C3	-2.3050506199	0.2138737486	0.1052791376
C4	-3.4870344736	0.9533512056	0.1049761622
C5	-4.7121966414	0.2726196912	0.0996813215
C6	-4.7492607898	-1.1391066106	0.0947418644
N7	-1.0013522090	0.6040840481	0.1097290970
C8	-0.1728809753	-0.5290904836	0.1078013212

C9	-0.9533307692	-1.7227394667	0.1018918457
O10	-0.5279771991	-2.9375877383	0.0988181384
C11	1.2285633116	-0.3769290731	0.1116135670
N12	2.0566839559	-1.5103941216	0.1095656583
C13	3.3604710959	-1.1205557867	0.1140181554
C14	3.3809561742	0.3257749598	0.1191931291
C15	2.0092974231	0.8165114307	0.1176582725
O16	1.5844029701	2.0314680871	0.1209478872
C17	4.5423055048	-1.8603074385	0.1142018831
C18	5.7676199891	-1.1798838877	0.1195553595
C19	5.8050736332	0.2318375481	0.1246808429
C20	4.6260386782	0.9738301442	0.1245038105
H21	-3.5902994013	-2.9684080251	0.0912537599
H22	-3.4561151087	2.0414131979	0.1087809830
H23	-5.6410422435	0.8390390463	0.0993757450
H24	-5.7118360785	-1.6485627028	0.0906635561
H25	-0.5707057687	1.5240220391	0.1139105958
H26	1.6253638329	-2.4301227998	0.1053021413
H27	4.5111081019	-2.9483621019	0.1102623828
H28	6.6963239521	-1.7465379089	0.1197638290
H29	6.7677876372	0.7410317515	0.1288083882
H30	4.6465305140	2.0614077867	0.1284533981

##### final #####